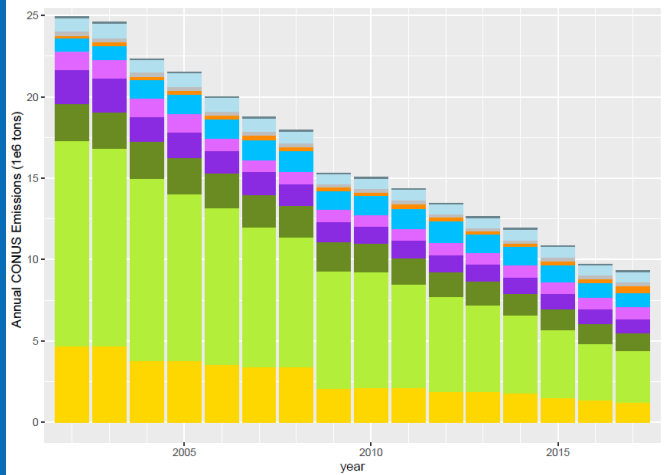


# EQUATES

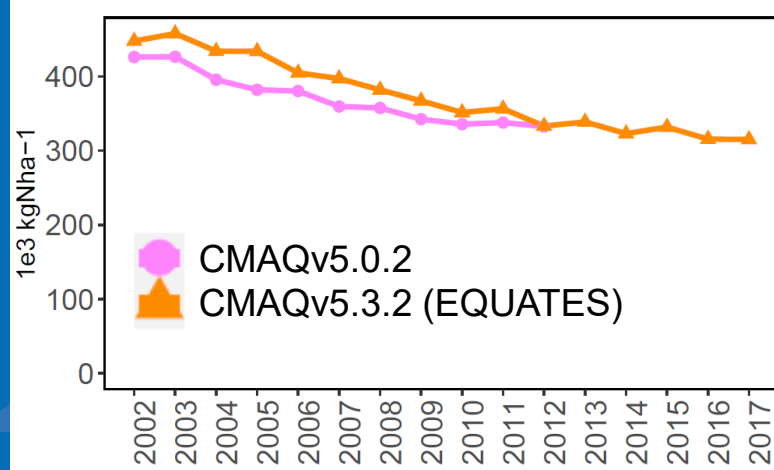
## EPA's Air QUALity Time Series Project

2002-2017 meteorology, emissions, and air quality modeling for the Northern Hemisphere and the Conterminous United States

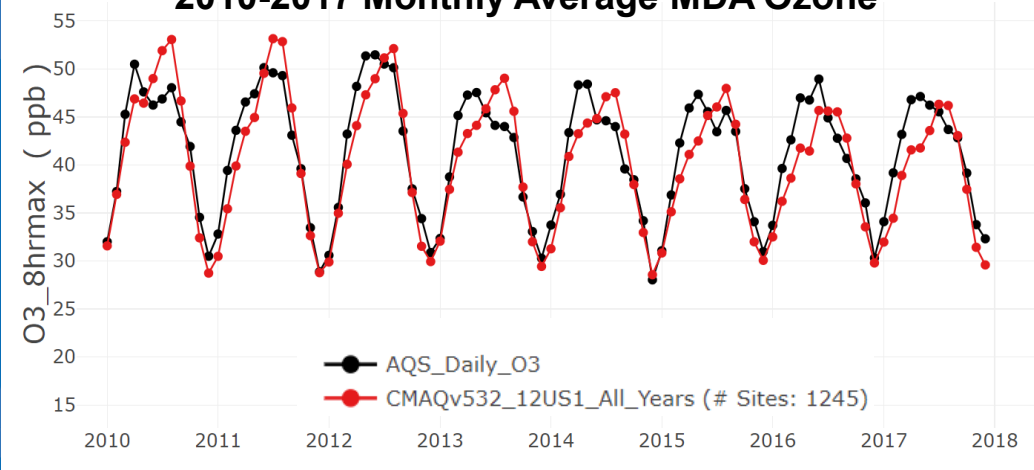
2002-2017 NO<sub>x</sub> Emissions



2002-2017 Total Nitrogen Deposition



2010-2017 Monthly Average MDA Ozone



Presented by Kristen Foley on behalf of the EQUATES Team

# EQUATES Team

- **Overall coordination:** Kristen Foley, George Pouliot, Alison Eyth, Norm Possiel
- **Meteorology modeling:** Rob Gilliam, Wyatt Appel, Jesse Bash, Brian Eder, Chris Misenis, Lara Reynolds
- **Emissions modeling:** Michael Aldridge, Chris Allen, Jesse Bash, Megan Beardsley, James Beidler, David Choi, Caroline Farkas, Janice Godfrey, Barron Henderson, Shannon Koplitz, Rich Mason, Rohit Mathur, Havala Pye, Matthew Roark, Sarah Roberts, Karl Seltzer, Darrell Sonntag, Kevin Talgo, Claudia Toro, Jeff Vukovich  
Additional emissions modeling support from ERG
- **CMAQ modeling:** Wyatt Appel, Christian Hogrefe
- **Evaluation, analysis, and data sharing:** Liz Adams, Wyatt Appel, Sarav Arunachalam, Jesse Bash, Sarah Benish, Barron Henderson, Christian Hogrefe, Shannon Koplitz, Rohit Mathur, Havala Pye, Donna Schwede, Karl Seltzer, Heather Simon

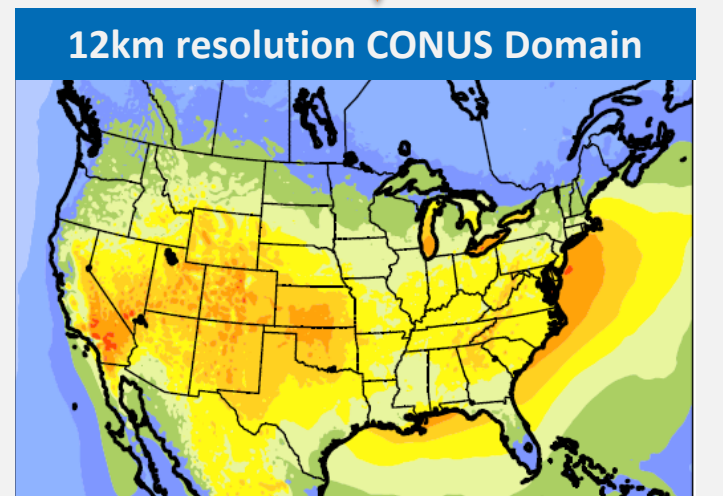
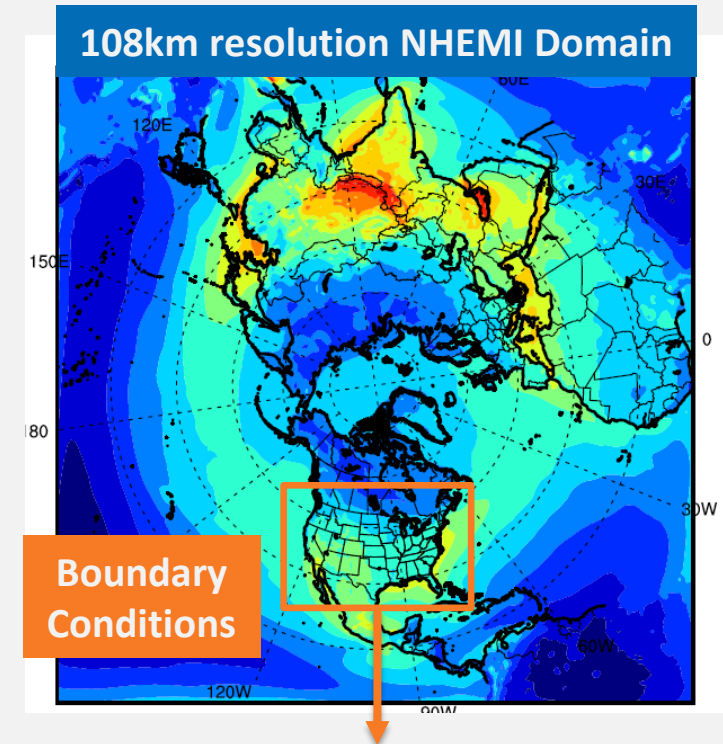
# *EQUATES Team*



# Overview of EQUATES Modeling Effort

**EQUATES provides a unified set of modeling data across applications**

- Temporal coverage: 2002-2017 (eventually 2018-2019)
- Spatial domains: Northern Hemisphere and contiguous US
- Meteorology inputs: New meteorological modeling for both domains using state-of-the-science retrospective simulations
- Emissions inputs: New inventories were developed using EPA's 2017 NEI as the base year with consistent methods used for each sector to avoid artificial step changes
- CMAQ version 5.3.2



# Motivation for EQUATES Project

- Decadal and multidecadal CMAQ simulations have been used for a wide variety of health and ecosystem applications



Critical loads  
and nutrient  
assessments



Epidemiological  
studies



Trends analysis  
and model  
evaluation

- Each set of simulations used a slightly different approach for modeling across years
  - “DOE” ([Xing et al., 2013](#); [Gan et al., 2015](#)): 1990-2010 CMAQv5.0.2 simulations at 36km resolution
  - “ECODEP” ([Zhang et al., 2019](#)): 2002 -2012 CMAQv5.0.2 simulations at 12km resolution
  - [EPA’s Fused Air Quality Surfaces](#): 2002-2017 model/observed ‘fused’ ozone and PM<sub>2.5</sub> surfaces using the best available modeling data and a Bayesian statistical downscaling model

# Multiyear CMAQ Simulations

	<b>CMAQv5.0.2 “DOE”</b> <a href="#">Xing et al. (2013)</a> <a href="#">Gan et al. (2015)</a>	<b>CMAQv5.0.2 “ECODEP”</b> <a href="#">Zhang et al. (2019)</a>	<b>FAQSD</b> <a href="#">Berrocal et al. (2012)</a>	<b>CMAQv5.3.2 “EQUATES”</b>
Model	CMAQv5.0.2 (CB05_AERO6; without bidirectional NH <sub>3</sub> )	CMAQv5.0.2 (CB05TUCL-AERO6; with bidirectional NH <sub>3</sub> )	Various CMAQ versions (v4.6-5.3)	<b>CMAQv5.3.2 (CB6R3-AERO7; with bidi NH<sub>3</sub>)</b>
Date range	1990 - 2010	2002 – 2012	2002-2017	<b>2002 – 2017 (+2018-2019)</b>
Domain/ Resolution	108km NHEMI + 36km CONUS	12km CONUS	12km CONUS	<b>108km NHEMI + 12km CONUS</b>
Meteorology	WRF3.4	WRF3.4	Various WRF versions	<b>WRFv4.1.1</b>
Emissions	NEI data (2002 or 2005 base year + scaling factors and emissions constraints; MOBILE6 mobile sources; climatological fires, no CMV)	Various NEIs / Modeling Platforms (2002-2011: MOVES2010b and 2012: MOVES2014a); year specific fires, CMV included	Various NEIs / Modeling Platforms	<b>2017 NEI as primary base year; consistent methods used for each sector (when feasible) to avoid artificial step changes</b>
Boundary Conditions	N Hemi CMAQv5.0.2	GEOS-Chem	Depends on the modeling year	<b>N Hemi CMAQv5.3.2</b>

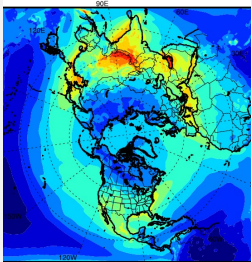
# Evaluation of New EQUATES Modeling



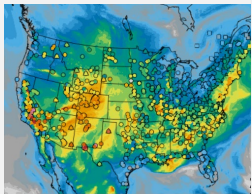
- **Meteorology** - See poster presentation by Rob Gilliam



- **Emissions** – comparison of EQUATES mobile, oil and gas, and fire emissions to previous emissions modeling platforms

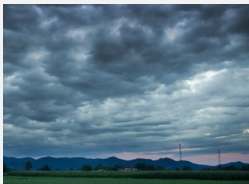


- **Hemispheric CMAQ** - See presentation by Christian Hogrefe in this session and poster presentation by Rebecca Miller



- **CMAQ over the US**
  - Initial evaluation of ozone, PM<sub>2.5</sub> and NO<sub>x</sub>
  - Deposition: See presentation by Sarah Benish in this session

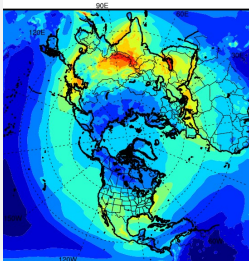
## For the topics covered in this talk, I will focus on success stories and remaining challenges



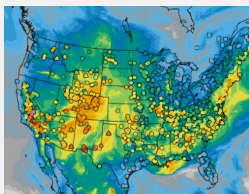
- **Meteorology** - See poster presentation by Rob Gilliam



- **Emissions** – comparison of EQUATES mobile, oil and gas, and fire emissions to previous emissions modeling platforms



- **Hemispheric CMAQ** - See presentation by Christian Hogrefe in this session and poster presentation by Rebecca Miller



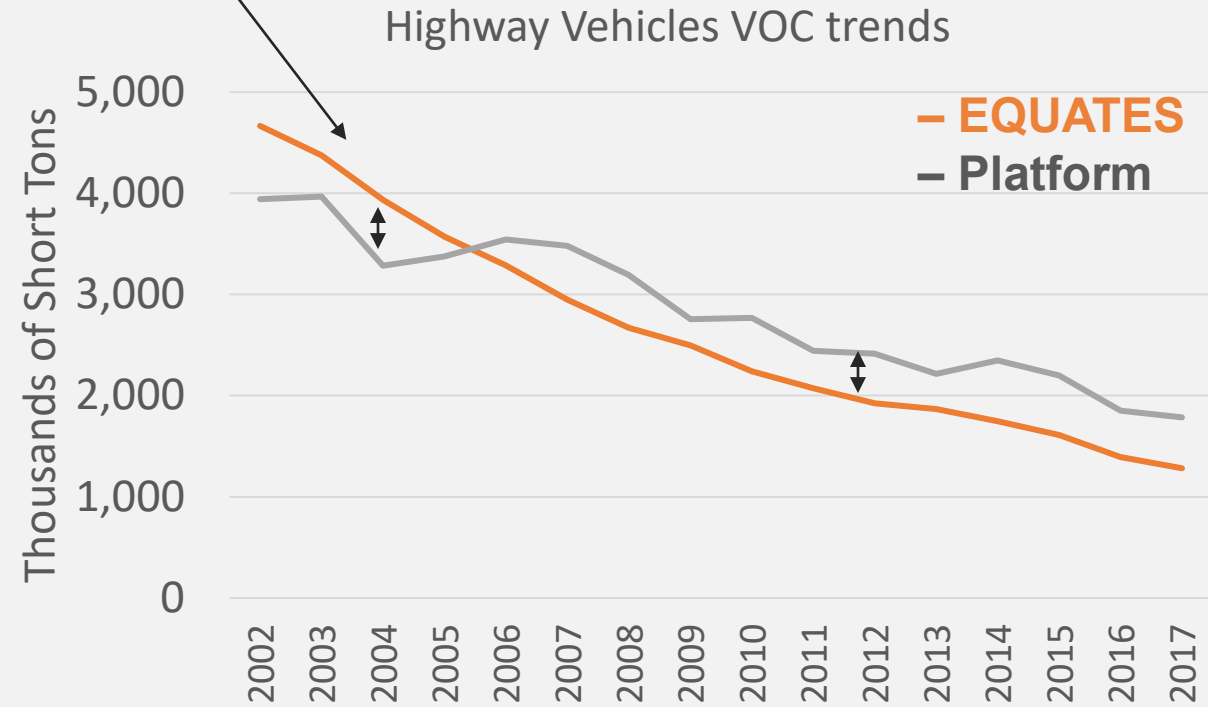
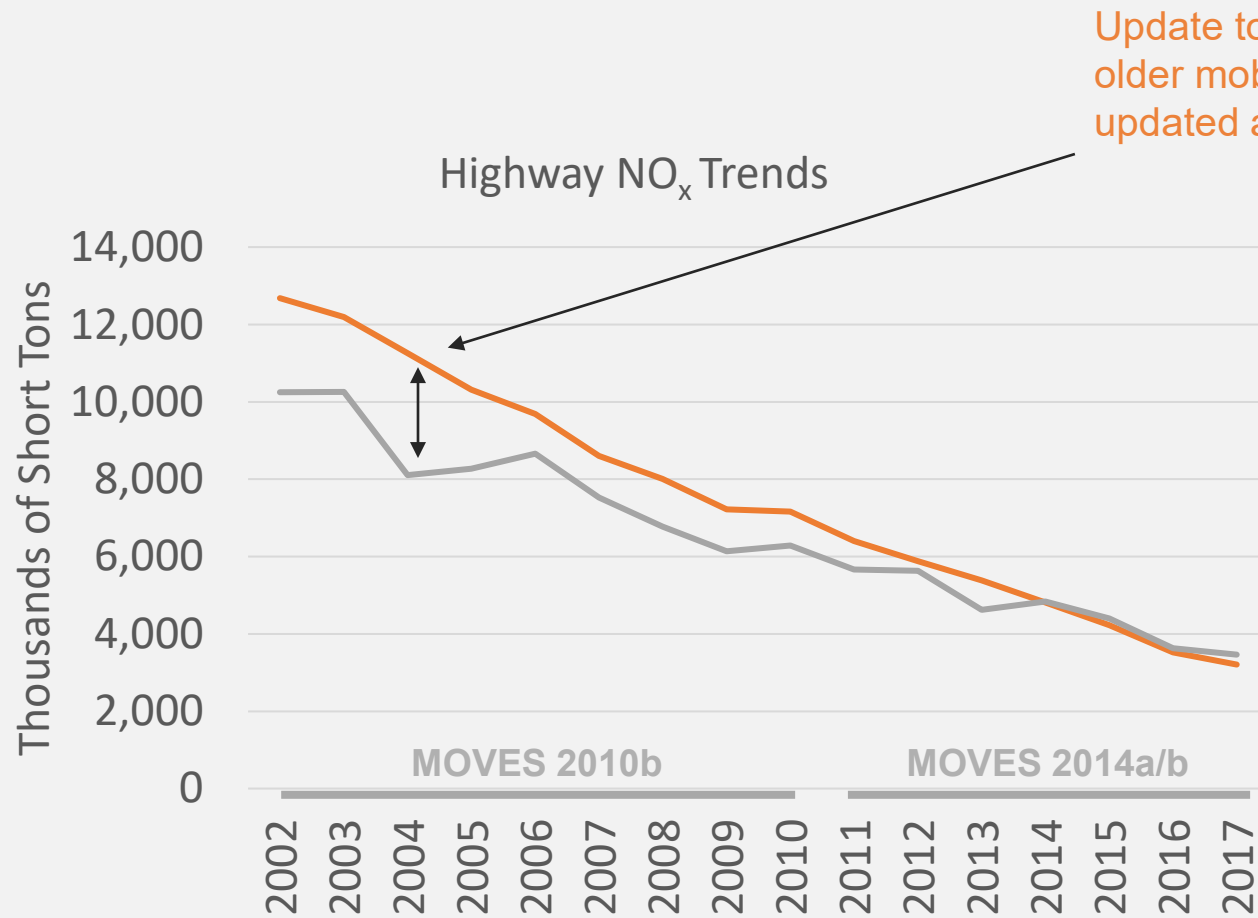
- **CMAQ over the US**
  - Initial evaluation of ozone,  $PM_{2.5}$  and  $NO_x$
  - Deposition: See presentation by Sarah Benish in this session



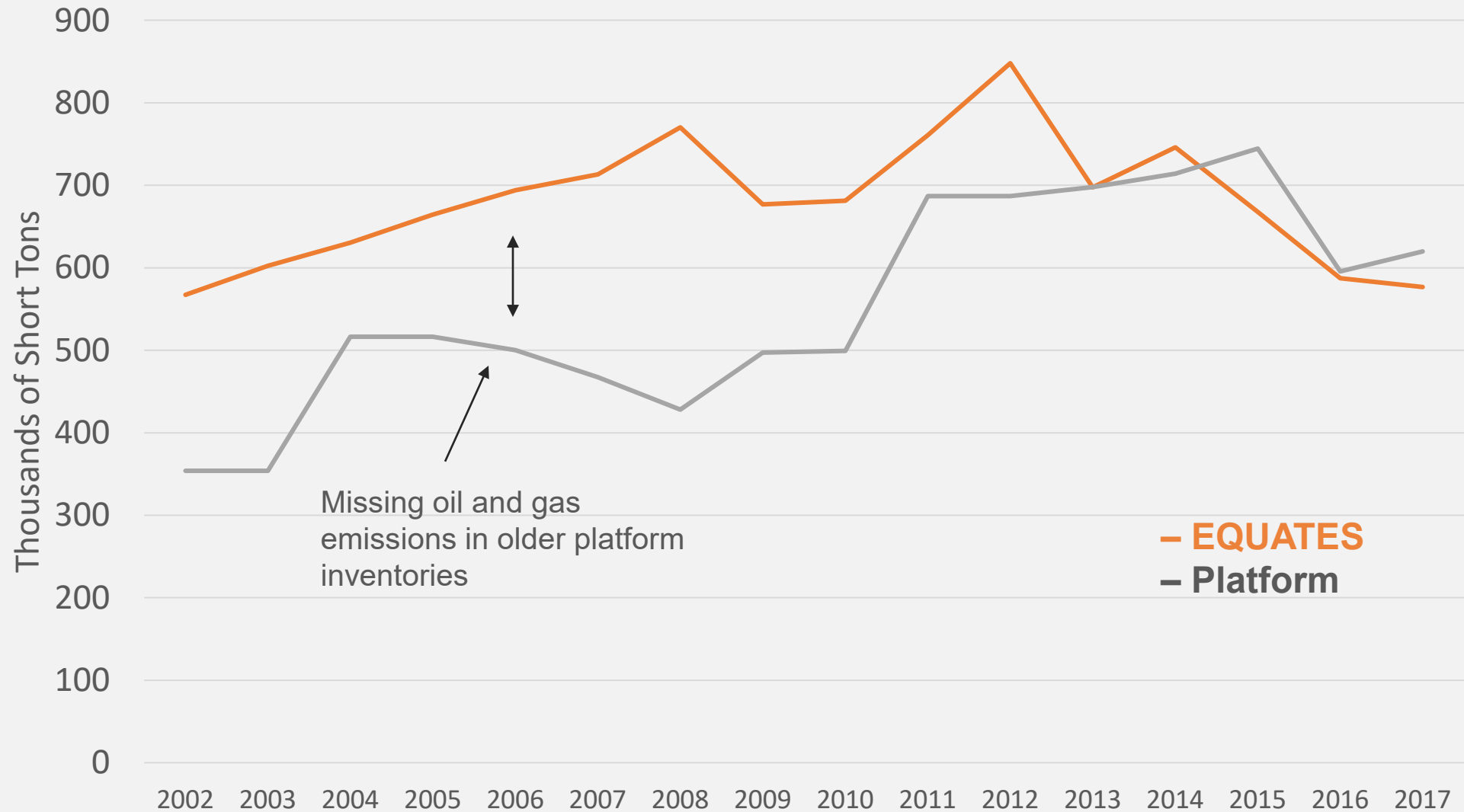
# Emissions Comparison

- The following slides highlight changes in EQUATES emissions in several important sectors: highway vehicles (onroad), oil and gas, and fire emissions
- We compare emissions trends from:
  - **EQUATES** inventory emissions (before SMOKE processing)
  - **Platform** inventories based on a mix of NEI's and emissions modeling platforms (see supplemental slide for more information)
- A high-level summary of the methods used for EQUATES CONUS emissions is provided in the supplemental slides.

# Highway NO<sub>x</sub> and VOC Emissions



# Petroleum and Related Industries NO<sub>x</sub> Emissions

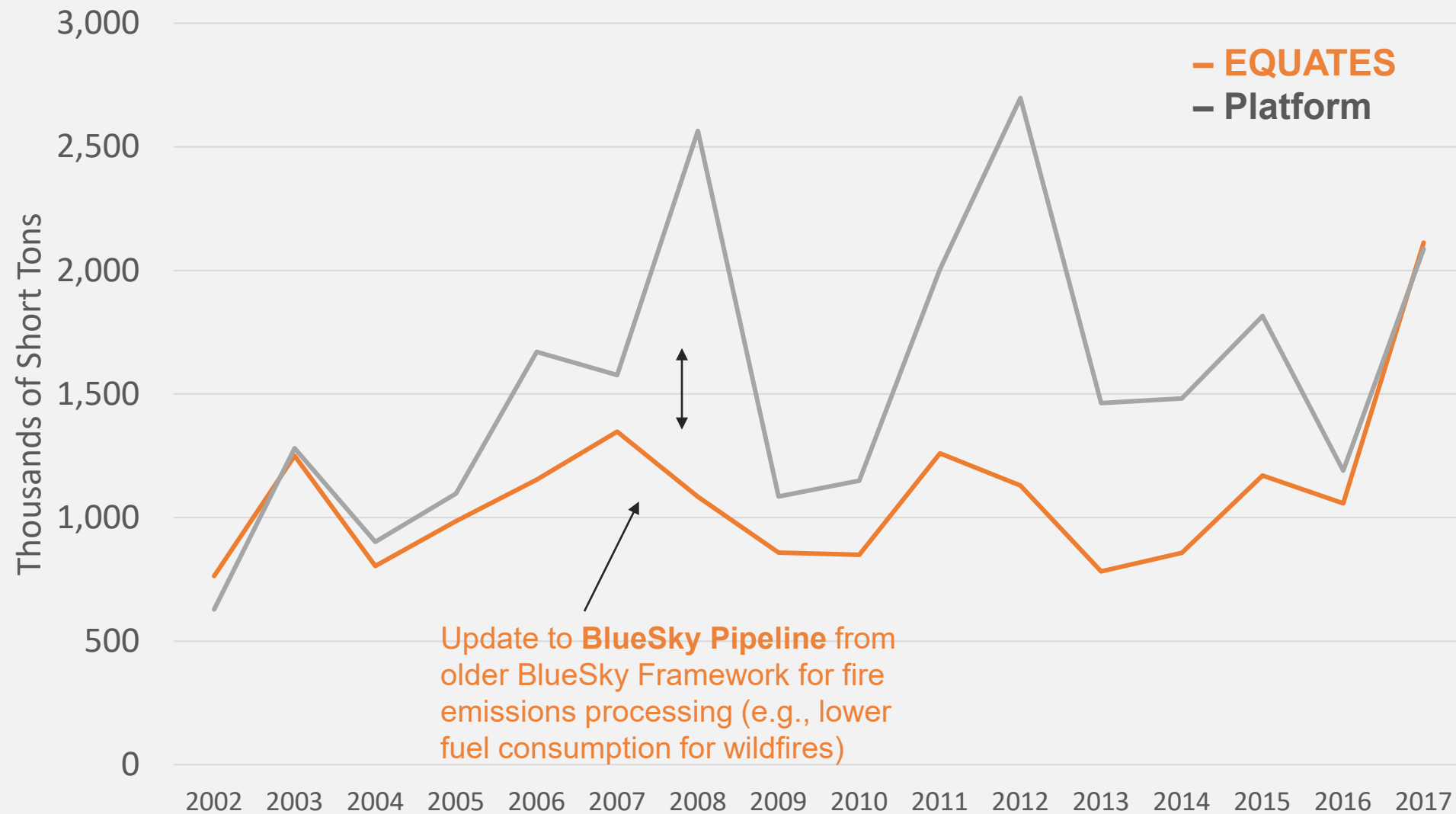


— EQUATES  
— Platform

Missing oil and gas  
emissions in older platform  
inventories

*EQUATES*

# Wildfires and Prescribed Fires PM<sub>2.5</sub> Emissions

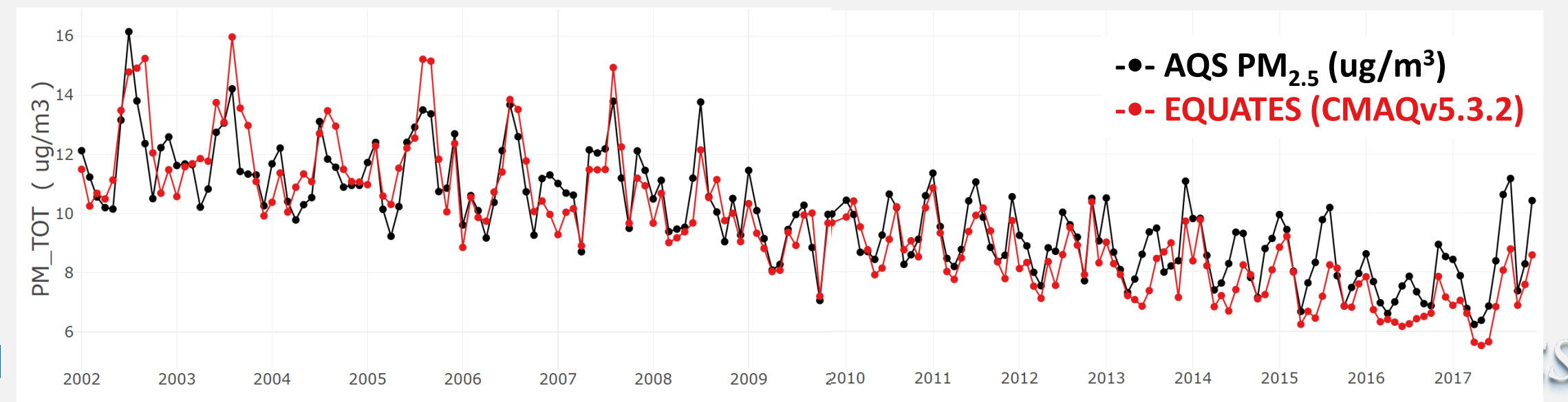
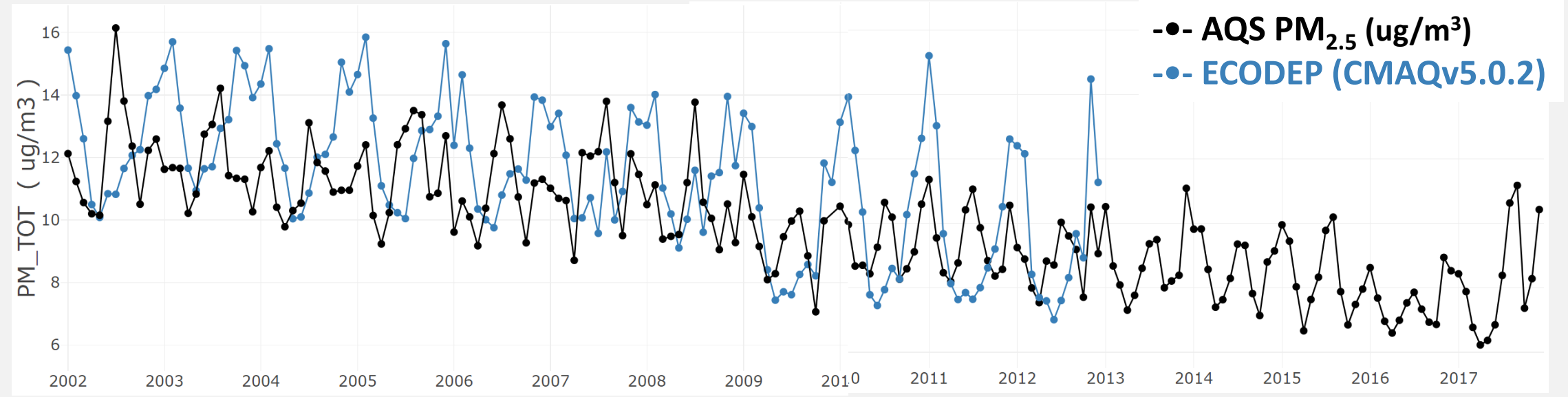


# CMAQ Evaluation: ECODEP vs EQUATES

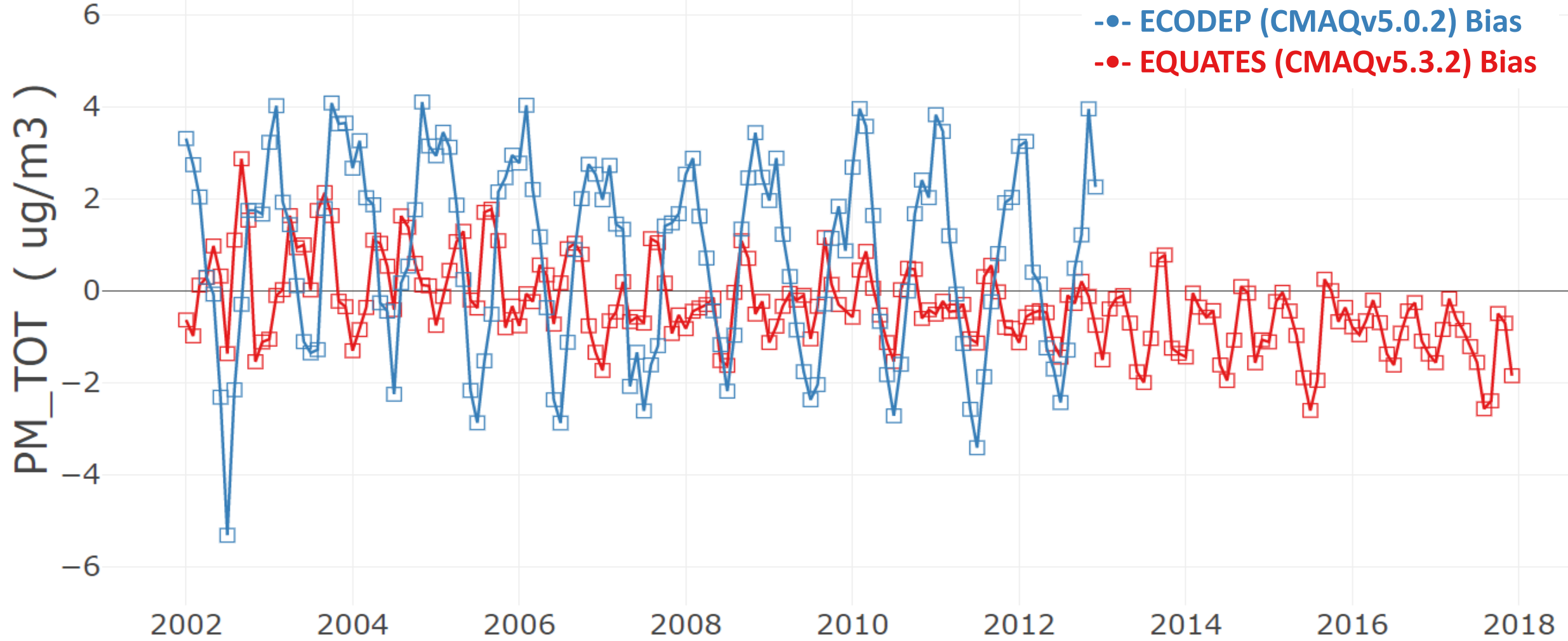
- The following slides show a few highlights of the evaluation of the **EQUATES** CMAQv5.3.2 simulations by comparing results from the **ECODEP** CMAQv5.0.2 simulations.
- We focus on  $PM_{2.5}$ , maximum daily 8-hr average ozone (MDA8  $O_3$ ), and  $NO_x$ .

**PM<sub>2.5</sub>**

# Seasonal Pattern in Monthly Average PM<sub>2.5</sub>

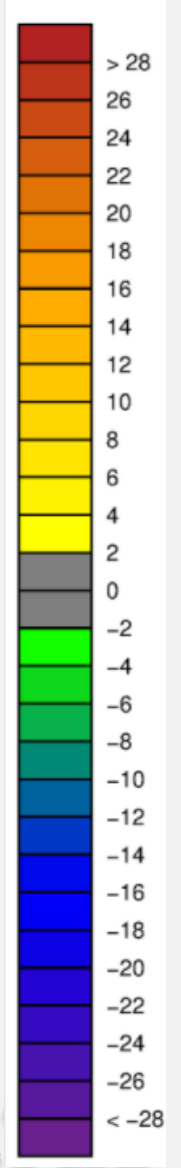
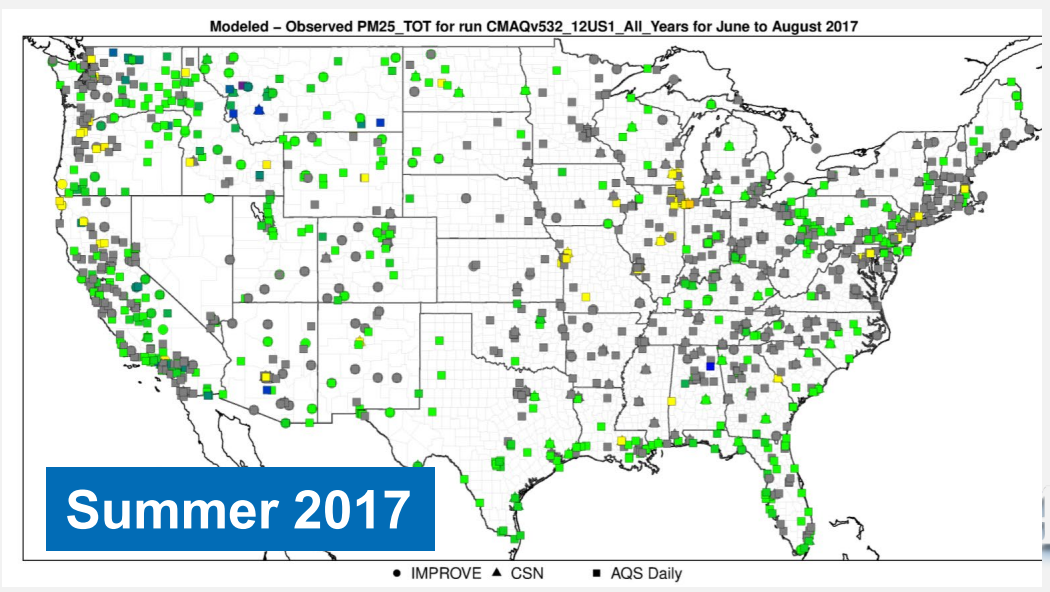
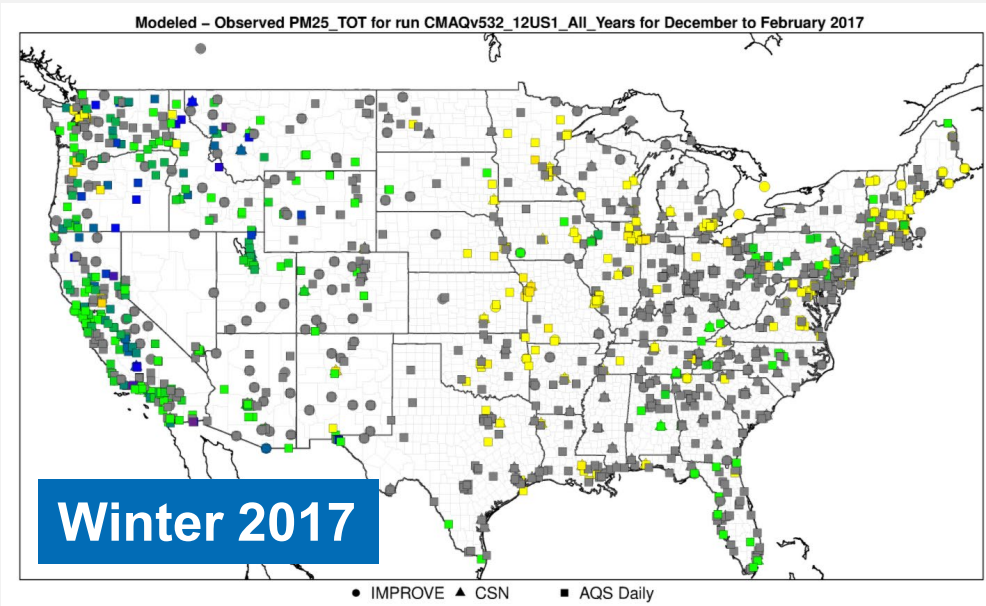
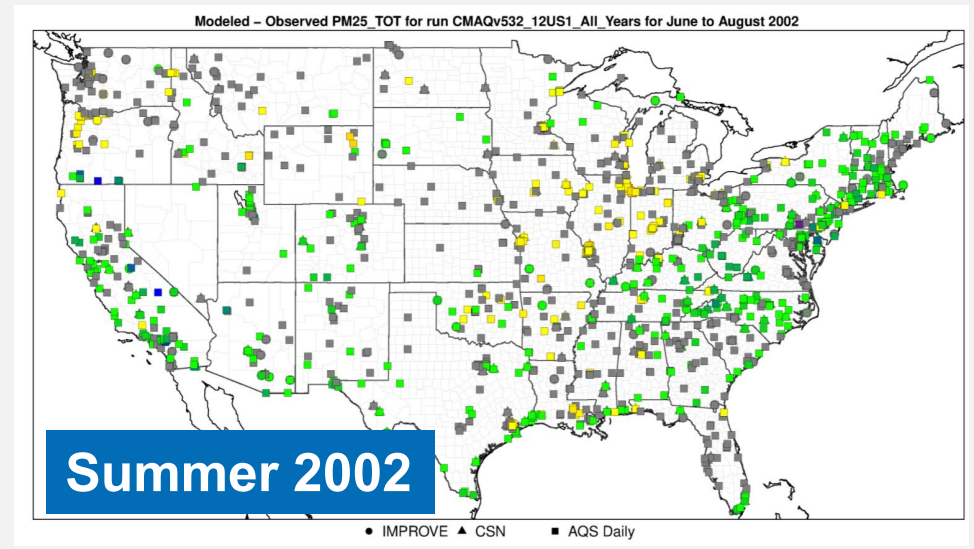
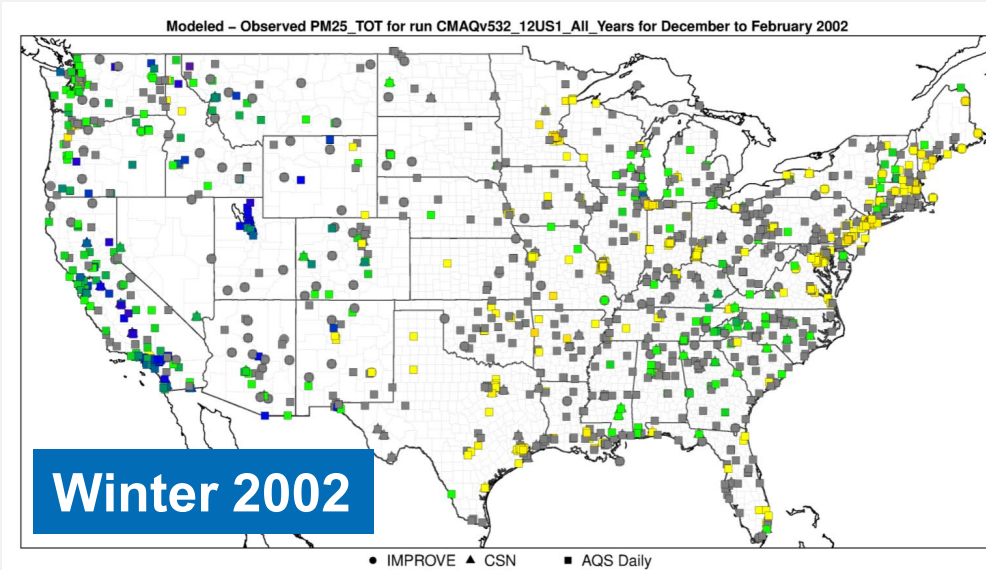


# 2002 - 2017 PM<sub>2.5</sub> Monthly Mean Bias



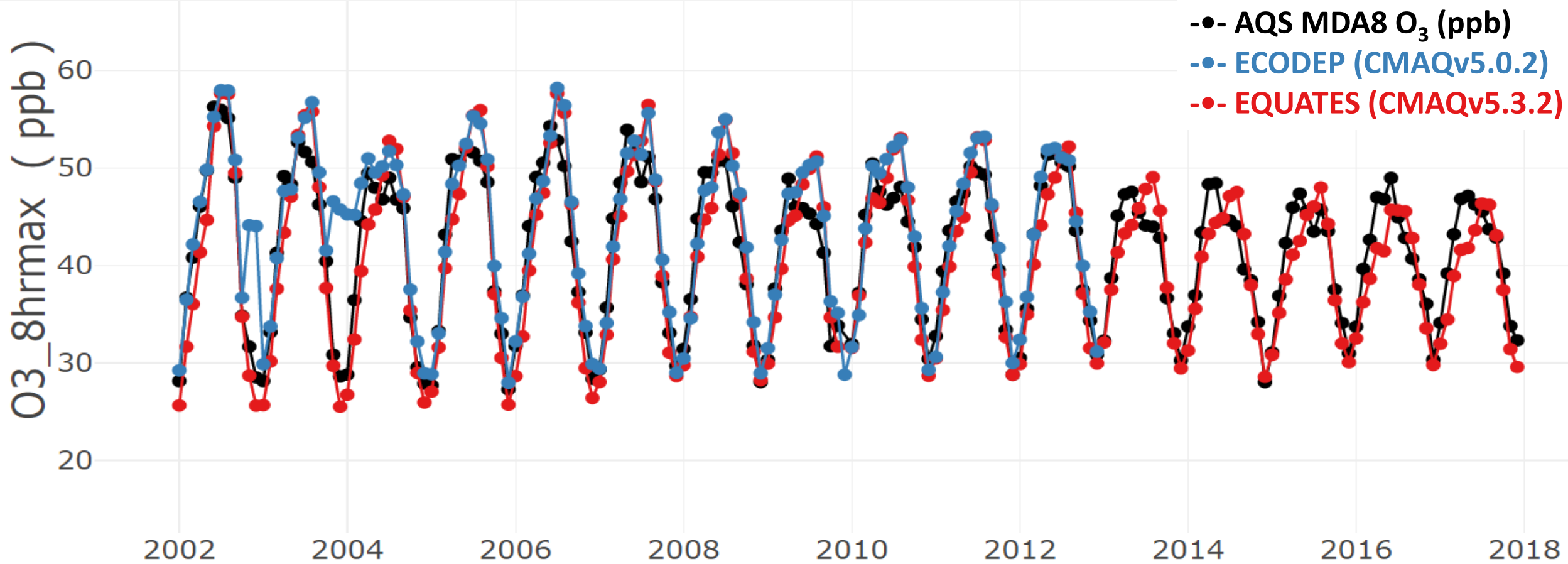


# EQUATES Winter/Summer Mean Bias in PM<sub>2.5</sub>

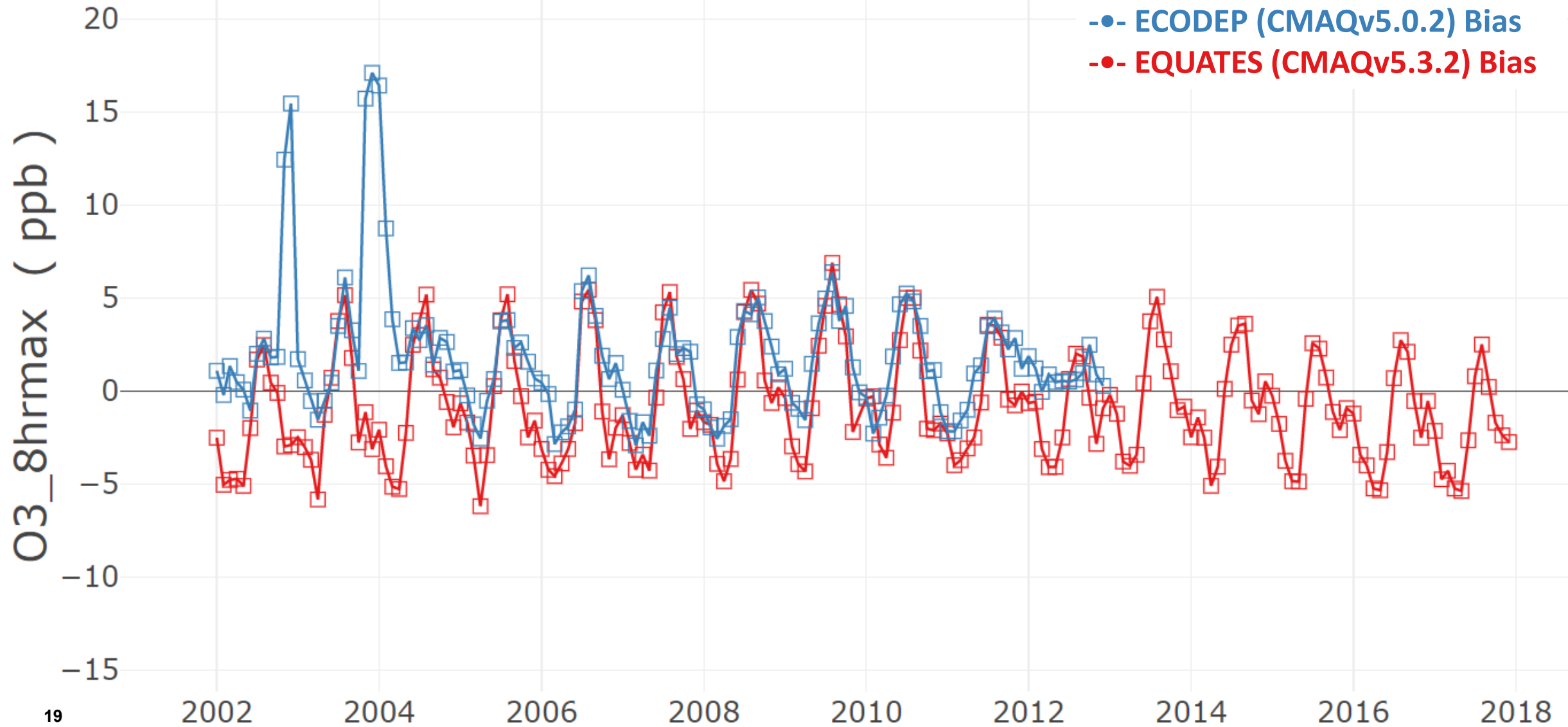


# Maximum Daily 8-hr Average Ozone

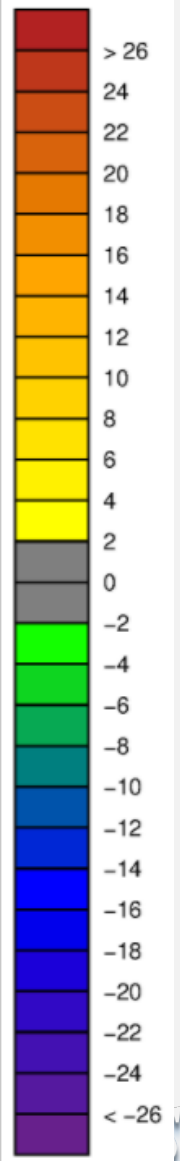
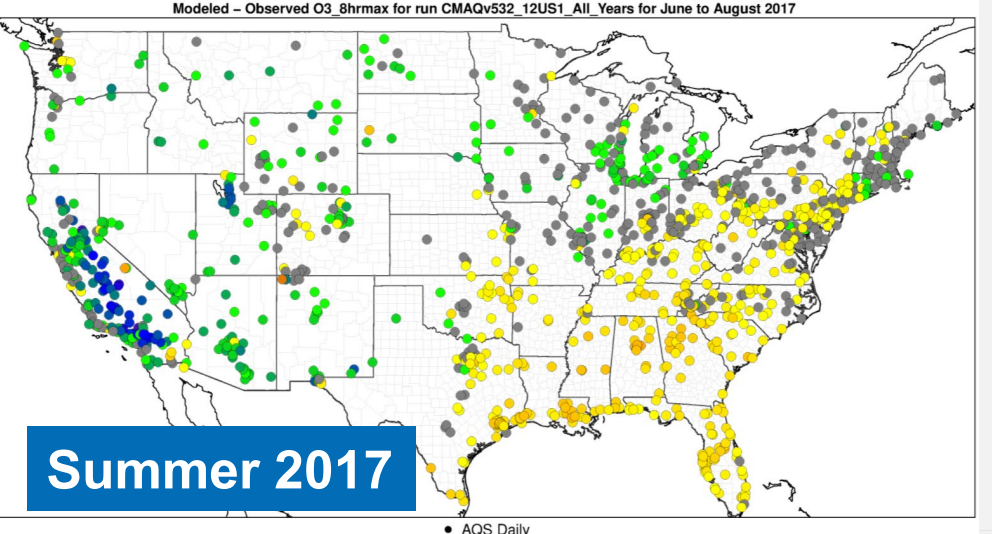
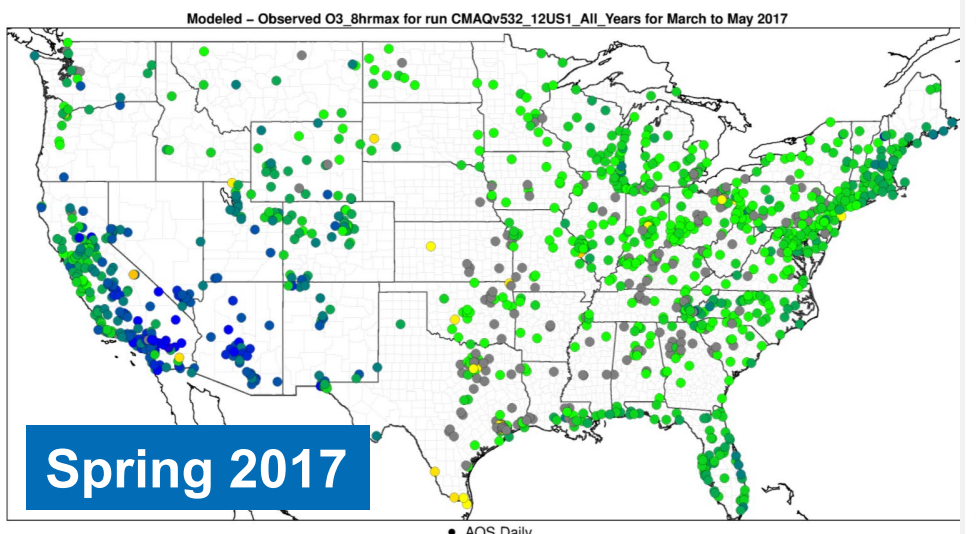
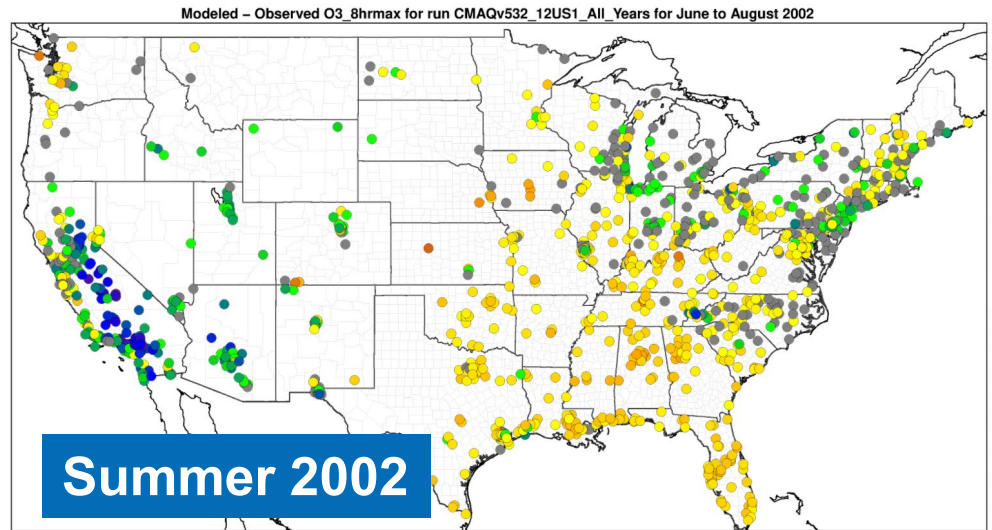
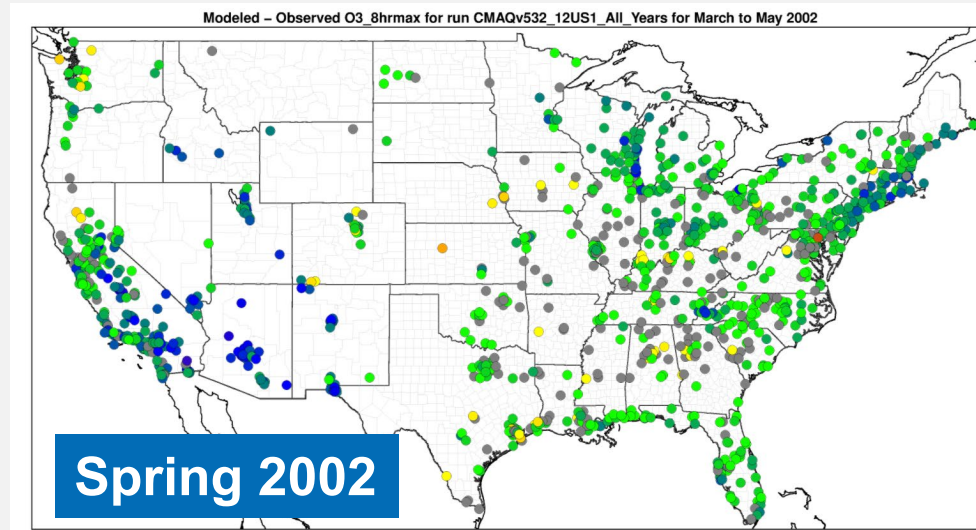
# 2002 - 2017 Seasonal Pattern in MDA8 O<sub>3</sub>



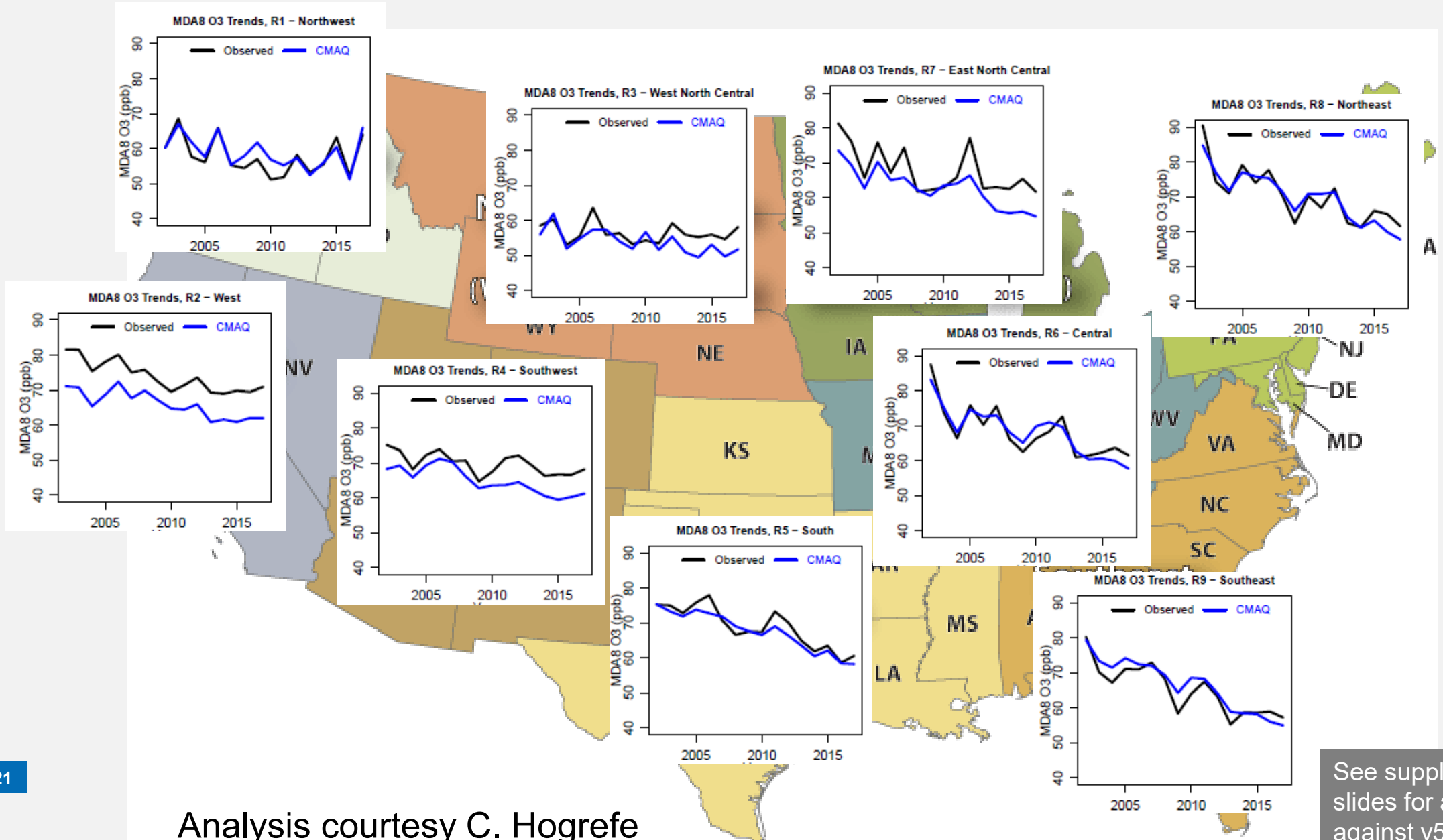
# 2002 - 2017 Seasonal Pattern in MDA8 O<sub>3</sub> Mean Bias



# EQUATES: Spring/Summer Mean Bias in MDA8 O<sub>3</sub>



# EQUATES: Trends in 95<sup>th</sup> Percentile MDA8 O<sub>3</sub> Ozone Season (May –Sept)

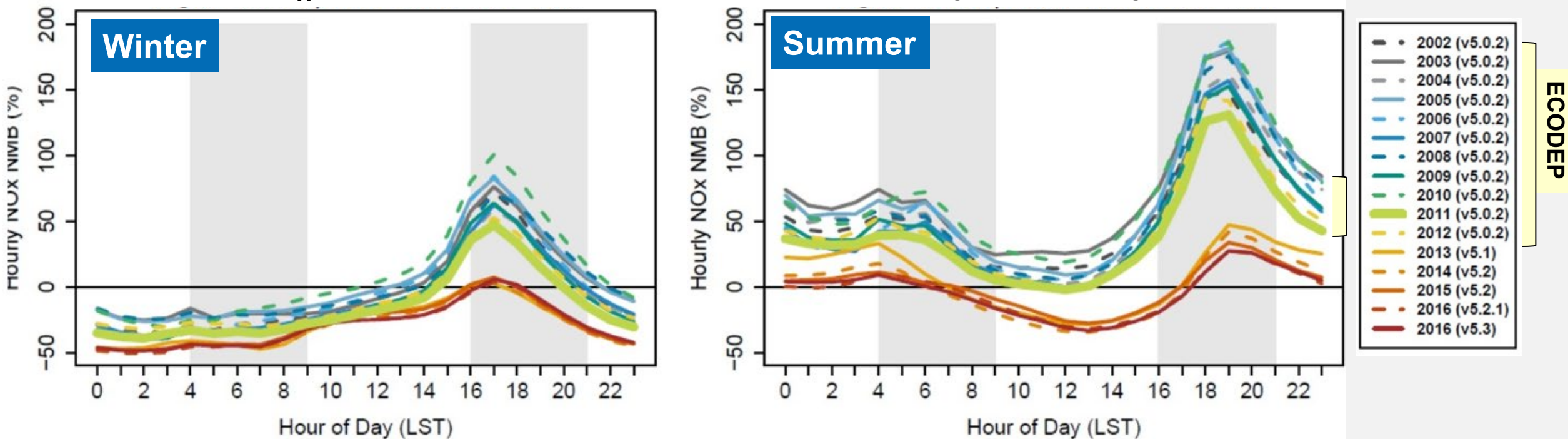


**NO<sub>x</sub>**

# ECODEP NO<sub>x</sub> Evaluation

- [Toro et al. \(2021\)](#) – Evaluation of NO<sub>x</sub> estimates from 2002-2016 CMAQ simulations. Figure 4 from the paper shows the diurnal pattern of the normalized mean bias in NO<sub>x</sub> at AQS sites in summer and winter.

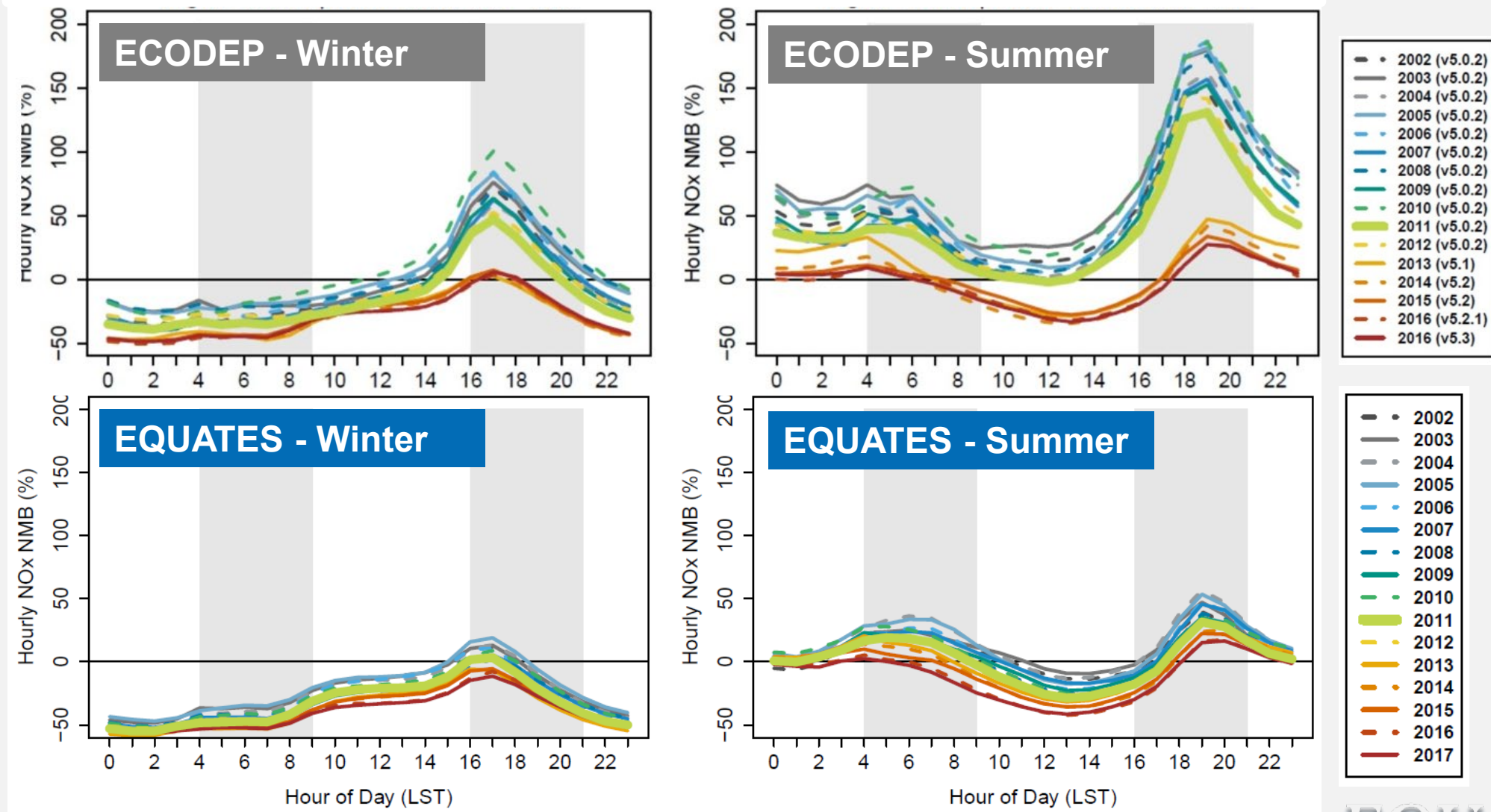
**NO<sub>x</sub> Normalized Mean Bias (%) Across All Sites by Hour of Day**





# ECODEP vs EQUATES NO<sub>x</sub> Evaluation

## NO<sub>x</sub> Normalized Mean Bias (%) Across All Sites by Hour of Day



See supplemental slides for a comparison of NO<sub>x</sub> evaluation across regions and seasons

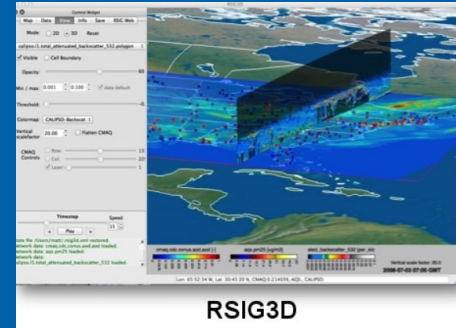
# EQUATES Data Sharing

- Initial data sharing effort is through the CMAS Data Warehouse
  - Emissions inventory files (SMOKE inputs)
  - CMAQ-ready meteorology, emissions, IC/BC input files for the 12US1 domain – including fertilizer inputs from EPIC to be used with the bidirectional NH<sub>3</sub> module in CMAQ
  - WRF evaluation datasets (matched model/obs data)
  - Daily average CMAQ output for the 12US1 domain for 14 pollutants
  - Daily average 3D CMAQ output for the 108NHEMI domain – can be used to create boundary conditions for domains within the N. hemisphere
- More data will be shared via other platforms in coming months

Visit [www.epa.gov/EQUATES](http://www.epa.gov/EQUATES) for more information

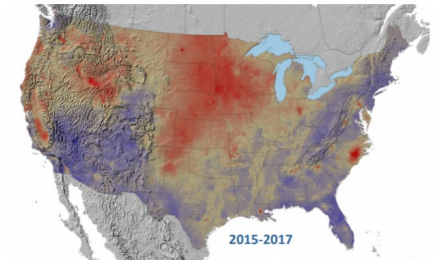


CMAS Data Warehouse



RSIG3D

2017 Total Deposition  
Measurement Model Fusion Maps



2015-2017



# Conclusions

- EQUATES provides a unified set of emissions, meteorology, and air quality modeling data for 2002-2017
- EQUATES emissions were developed using the latest tools and datasets to reduce step changes that can occur between NEIs due to changes in methods and input data
- CMAQ evaluation compared to previous timeseries:
  - Seasonality of PM<sub>2.5</sub> estimates is greatly improved
  - Summer NO<sub>x</sub> bias is greatly decreased
  - Underestimation that needs further diagnostic evaluation: wintertime PM<sub>2.5</sub>, springtime ozone, 95<sup>th</sup> percentile ozone in recent years, wintertime NO<sub>x</sub>
- EQUATES modeling datasets have been made publicly available to support additional analysis and evaluation

For more information on the slides in this presentation, please contact:

Kristen Foley (EPA/ORD/CEMM)

[Foley.Kristen@epa.gov](mailto:Foley.Kristen@epa.gov)

Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA.

# Supplemental Slides

**QA/POST-PROCESSING/EVALUATION**

**EQUATES**

**CONUS**

**N. HEMISPHERE**

**N. American Emissions Inventories (Modeling Platforms, Custom data)**

**Regional Meteorology Inputs**

**Emissions Modeling**  
MOVES, SMOKE, EPIC

**CONUS Meteorology Modeling**  
WRF+MCIP

**Regional Chemistry Transport Modeling**  
CMAQv5.3.2

**Boundary Conditions**

**Hemispheric Emissions Inventories (HTAP, CEDS, NEI data)**

**Hemispheric Meteorology Inputs**

**Emissions Modeling**  
SMOKE

**Hemispheric Meteorology Modeling**  
WRF+MCIP

**Hemispheric Chemistry Transport Modeling**  
CMAQv5.3.2

- Applications**
- Emissions and AQ Trends
  - Deposition Maps
  - Nutrient Assessments
  - Fused Surfaces
  - Health Studies
  - Background Ozone and PM<sub>2.5</sub>
  - Model Evaluation

# EQUATES CONUS Emissions Methods Table

Source	Category Name(s)	Brief Method Description
Agriculture	ag	NH3 fertilizer emissions estimated online in CMAQ. All other emissions based on scaling 2017 NEI values based on USDA animal head counts.
Electrical Generating Units	ptegu, cem	Use existing data (from multiple NEIs) for all years but processed using most recent tools/methods.
Fires	ptfire, ptfire_grass, ptagfire	Based on new methods ( <a href="#">Pouliot, 2020 CMAS presentation</a> )
Fugitive Dust	afdust	For ag dust, unpaved road dust, and paved road dust, use 2017 NEI data and scaling factors based on activity surrogates. All other sources use 2017 NEI data for all years
Mobile – Airports	airports	Use 2017 NEI data and scaling factors based on FAA Terminal Area Forecast data
Mobile - Commercial Marine Vessels	cmvc1c2, cmvc3	Use 2017 NEI data and scaling factors based on regional fuel consumption as an activity surrogate with additional pollutant-specific adjustments for fuel standards
Mobile – Nonroad	nonroad_gas, nonroad_diesel	Estimated using MOVES2014b supplemented with new data for CA and TX
Mobile – Onroad	onroad_gas, onroad_diesel	Estimated using MOVE3 supplemented with new data for CA
Mobile - Rail	rail	Use 2017 NEI data and scaling factors based on fuel sales data as an activity surrogate with additional adjustment for specific pollutants to account for regulation and sulfur technology
Oil and Gas	pt_oilgas	Use year-specific modeling platform data (based on multiple NEIs)
Oil and Gas	np_oilgas	Oil and Gas Tool
Other Nonpoint Sources -Commercial Cooking	nonpt	Use year-specific modeling platform data (based on multiple NEIs)
Other Nonpoint Sources -Fuel Combustion	nonpt	Commercial and Industrial Biomass use 2017 NEI data and scaling factors based on national-level consumption data. For all other emissions use year-specific modeling platform data (based on multiple NEIs).
Other Nonpoint Sources - Gas Stations	nonpt	Linear interpolation between 2002 and 2017 modeling platform data
Other Nonpoint Sources - Industrial Processes	nonpt	Use year-specific modeling platform data (based on multiple NEIs)
Other Nonpoint Sources - Miscellaneous	nonpt	2017 NEI data for all years
Other Nonpoint Sources - Waste Disposal	nonpt	Use 2017 NEI data for all years, except composting. For composting scale 2017 NEI values based on activity surrogate.
Other Point Sources - Fuel Combustion	ptnonipm	Use year-specific modeling platform data (based on multiple NEIs)
Other Point Sources - Gas Stations	ptnonipm	Linear interpolation between 2002 NEI and 2017 NEI data.
Other Point Sources - Industrial Processes	ptnonipm	Use year-specific modeling platform data (based on multiple NEIs)
Other Point Sources - Miscellaneous	ptnonipm	2017 NEI data for all years
Other Point Sources - Waste Disposal	ptnonipm	Use 2017 NEI data for all years, except composting. For composting scale 2017 values based on activity surrogate.
Residential Wood Combustion	rwc	Scale 2017 NEI values based on national-level consumption data
Volatile Chemical Products including Solvents	np_solvents	Based on new method ( <a href="#">Seltzer et al., 2021</a> )

# Pre-SMOKE Emissions for Platform Case

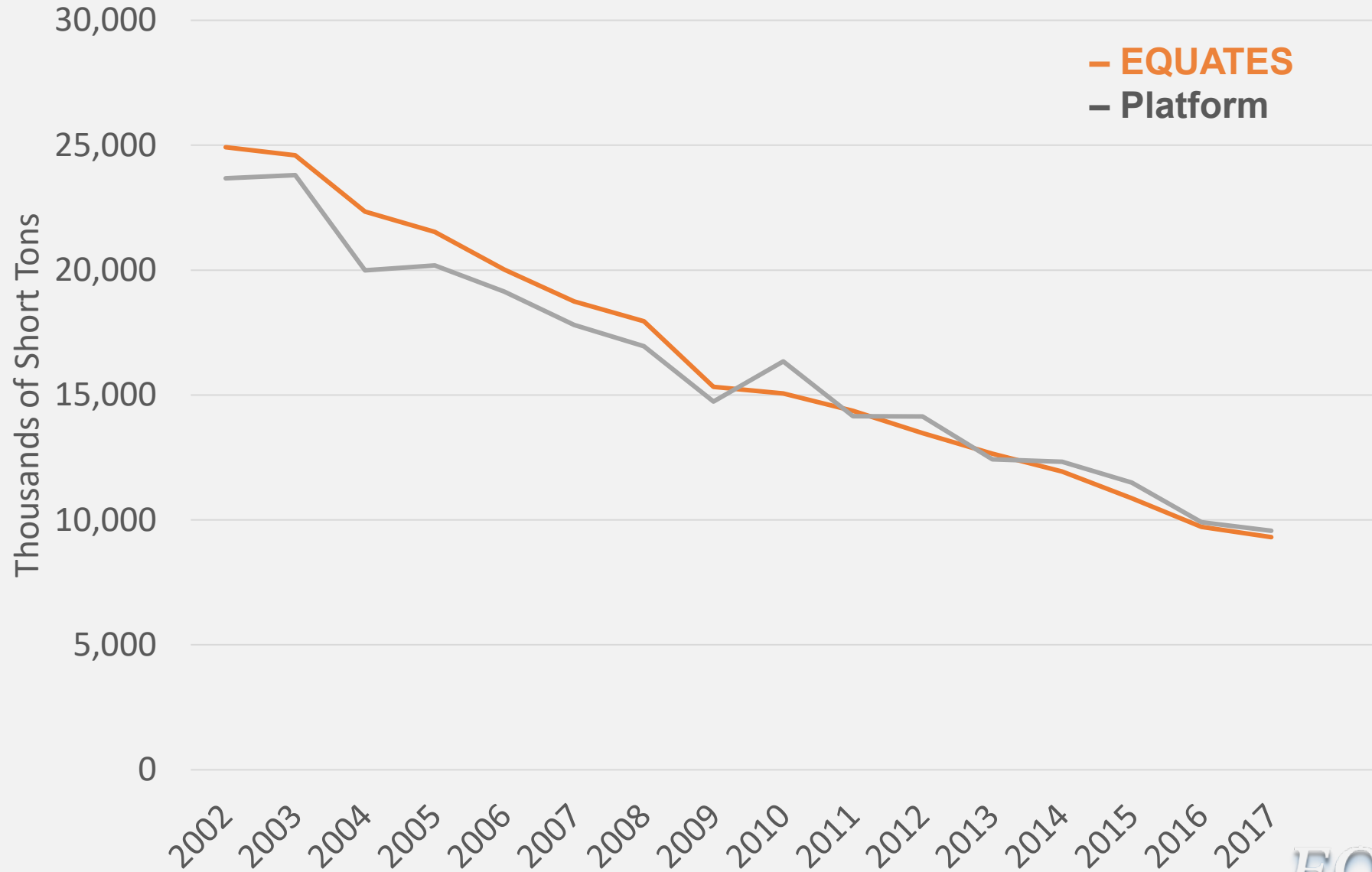
- Pre-SMOKE annual CONUS emissions totals for **Platform Case**:
  - Emissions modeling platform data used for 2002-2012 CMAQv5.0.2 simulations (“ECODEP”)
  - Additional emissions modeling platform data for 2013-2017
  - Platform data are based on several different NEIs and include substantial methods changes across the 16 years

ECODEP

Year	NEI	Emission Case	based on OAQPS case
2002	2002 NEI v3	E40 2002af	2005ct_ldghg_05b LDGHG Base
2003	2002 NEI v3	E40 2003af CB05	2005ct_ldghg_05b LDGHG Base
2004	2005 NEI v3	E40_2005ct_04	2005ct_ldghg_05b LDGHG Base
2005	2005 NEI v3	E40_2005ct	2005ct_ldghg_05b LDGHG Base
2006	2008 NEIv3	E40 2007ed_06 CB05	2007ed_v5_07c Shakeout Run4
2007	2008 NEIv3	2007ec	2007ec
2008	2008 NEIv3	F40_2008ab	2008aa_08c CDC
2009	2008 NEIv3	F40_2009ef	2009ef_v5_09d CDC
2010	2008 NEIv3	E40 2007ed_10	2007ed_v5_07c Shakeout Run4
2011	2011 NEIv1	2011ed	
2012	2011 NEIv1	2011ed_12	
2013	2011 NEIv2 with updates	2013ek_cb6cmaq	2013ek_cb6cmaq_v6_11g
2014	2014 NEIv2 / 2016 alpha	2014fd_cb6_14j	2014fd_cb6_14j 2014v2 for CB6 CMAQ
2015	2014 NEIv2 / 2016 alpha+	2015fe_cb6_15j	2015fe_cb6_15j CDC 2015
2016	2014 NEIv2 / 2016 v1	2016fh_16j v1	2016fh_16j version 1 platform
2017	2017 NEIv1		



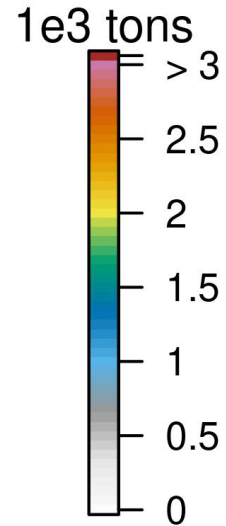
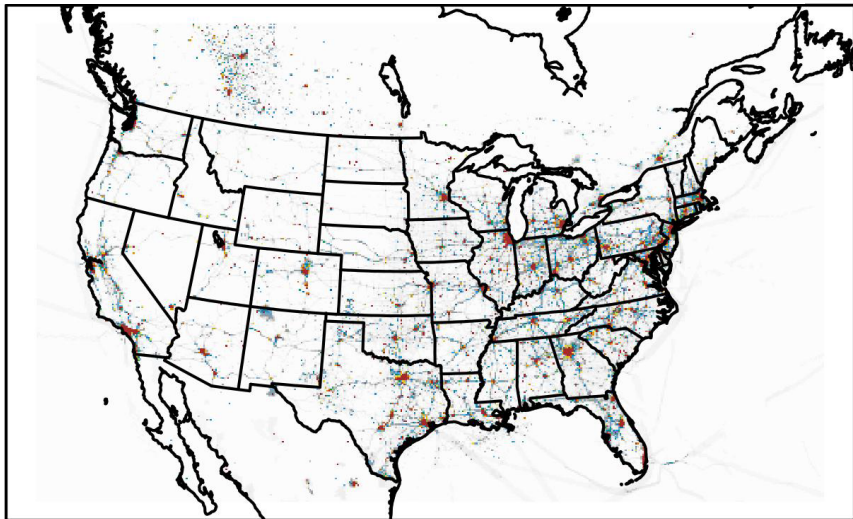
# NO<sub>x</sub> Anthropogenic Emissions



*EQUATES*

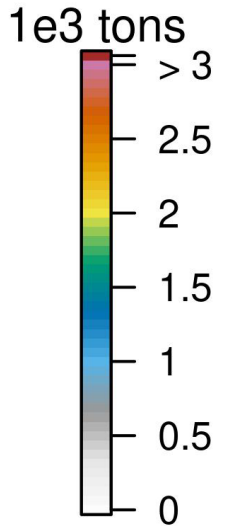
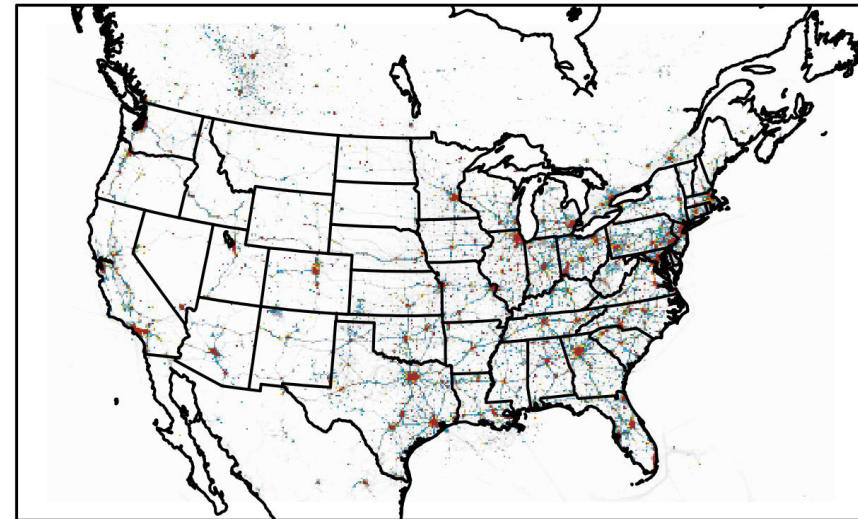
# ECODEP vs EQUATES: 2002 Anthropogenic NO<sub>x</sub> Emissions

### 2002 ECODEP NO<sub>x</sub> Emissions



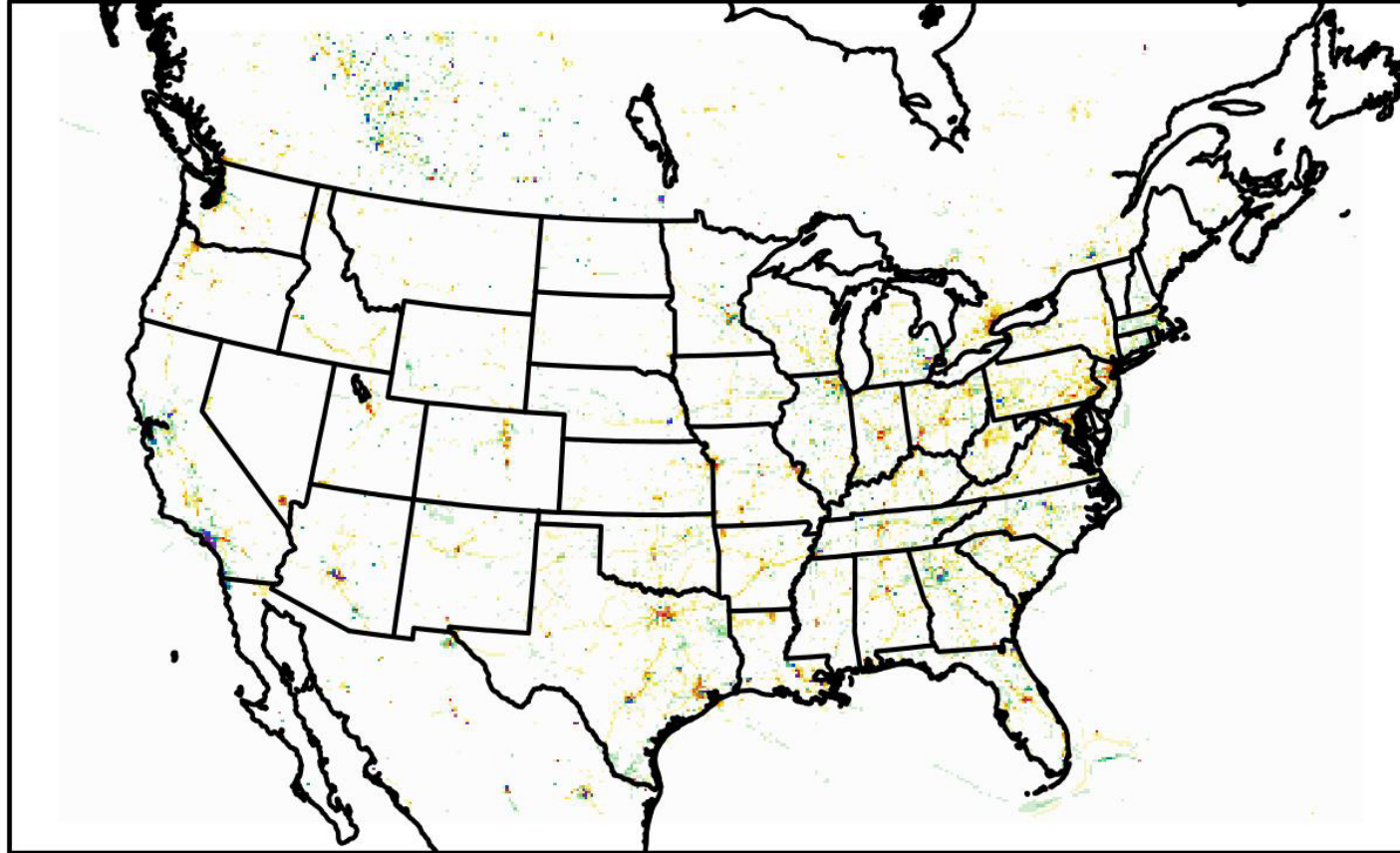
Domain size: 299x459 | Max = 120 at (38, 182)  
Mean: 0.21 | Median: 0.012

### 2002 EQUATES NO<sub>x</sub> Emissions

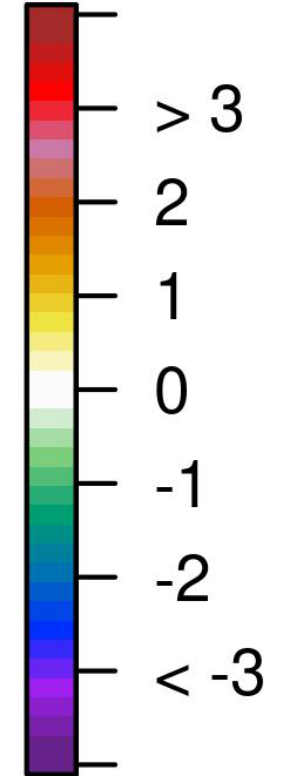


Domain size: 299x459 | Max = 70 at (143, 320)  
Mean: 0.21 | Median: 0.011

## EQUATES – ECODEP NO<sub>x</sub> 2002 Emissions

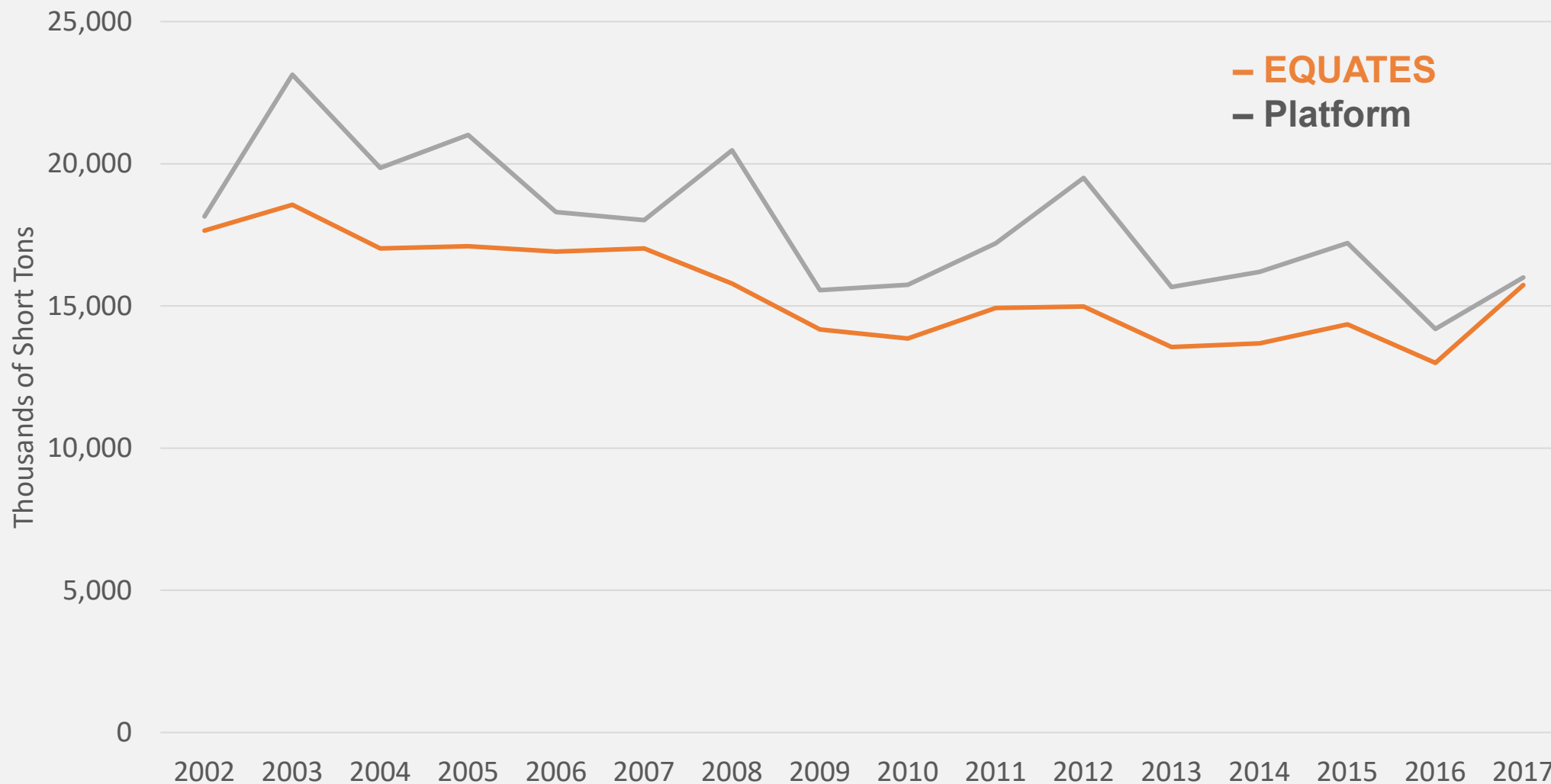


1e3 tons



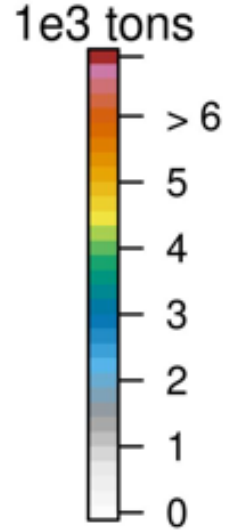
Min = -120 | Max = 28

# VOC Anthropogenic Emissions

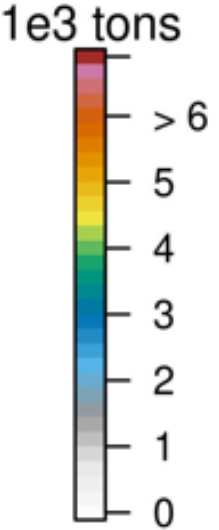


# ECODEP vs EQUATES: 2002 Anthropogenic VOC Emissions

## 2002 ECODEP VOC Emissions



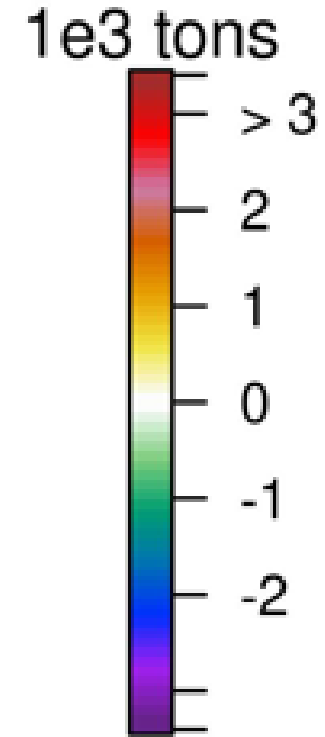
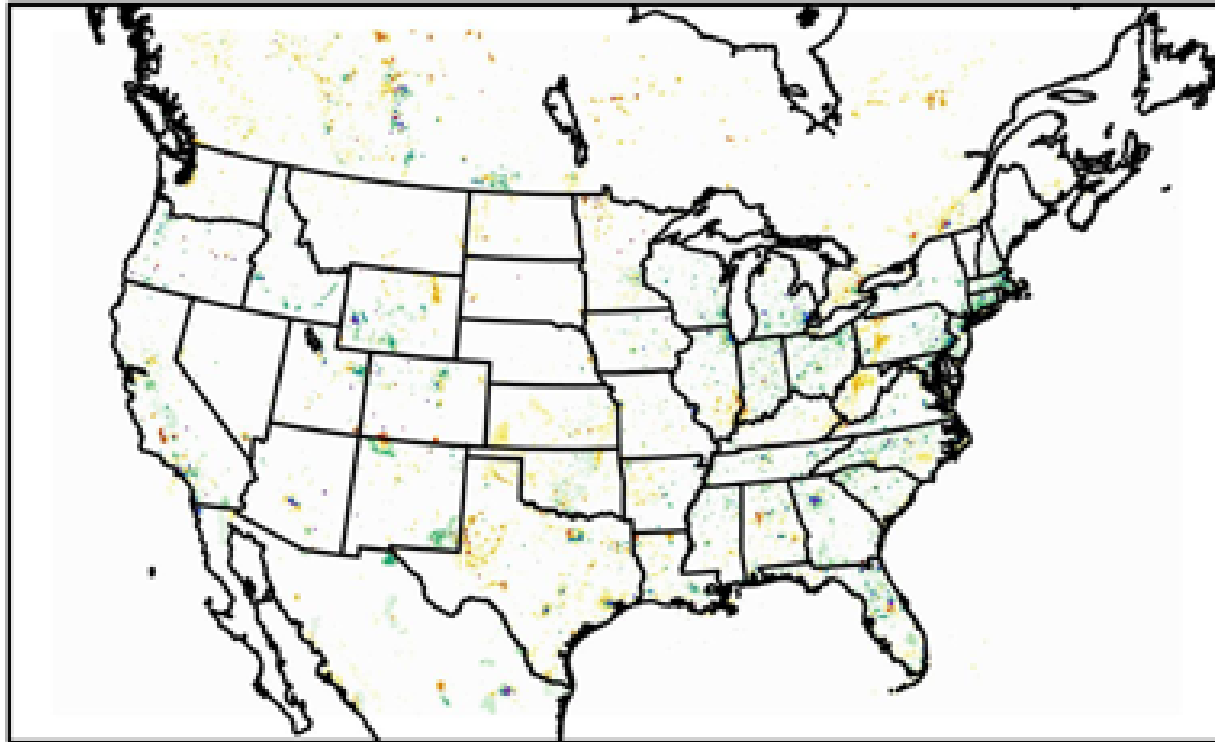
## 2002 EQUATES VOC Emissions



Domain size: 299x459 | Max = 150 at (194, 33)  
Mean: 0.12 | Median: 0.0054

Domain size: 299x459 | Max = 110 at (194, 33)  
Mean: 0.11 | Median: 0.005

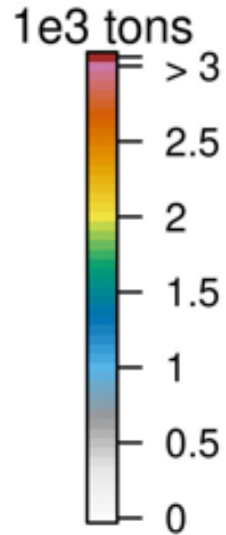
## EQUATES – ECODEP VOC 2002 Emissions



Min = -69.2 | Max = 24.9  
Mean: -0.00435 | Median: 1.01e-05

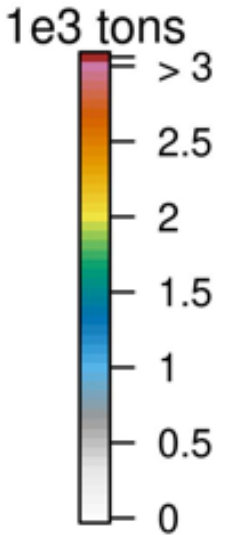
# ECODEP vs EQUATES: 2008 PM<sub>2.5</sub> Emissions

### 2008 ECODEP PM<sub>2.5</sub> Emissions



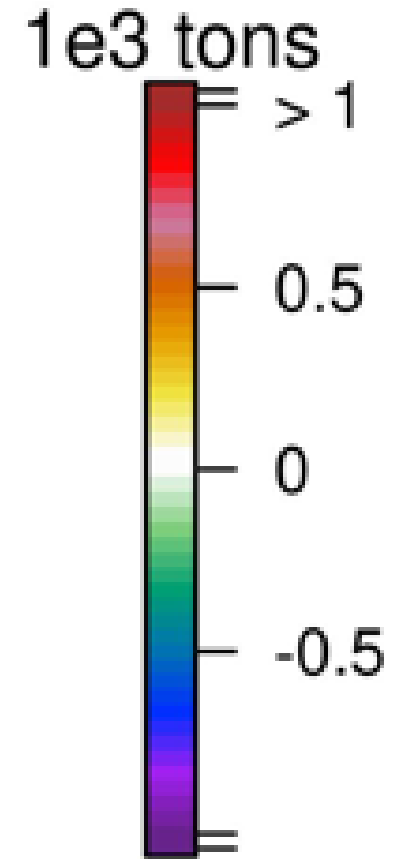
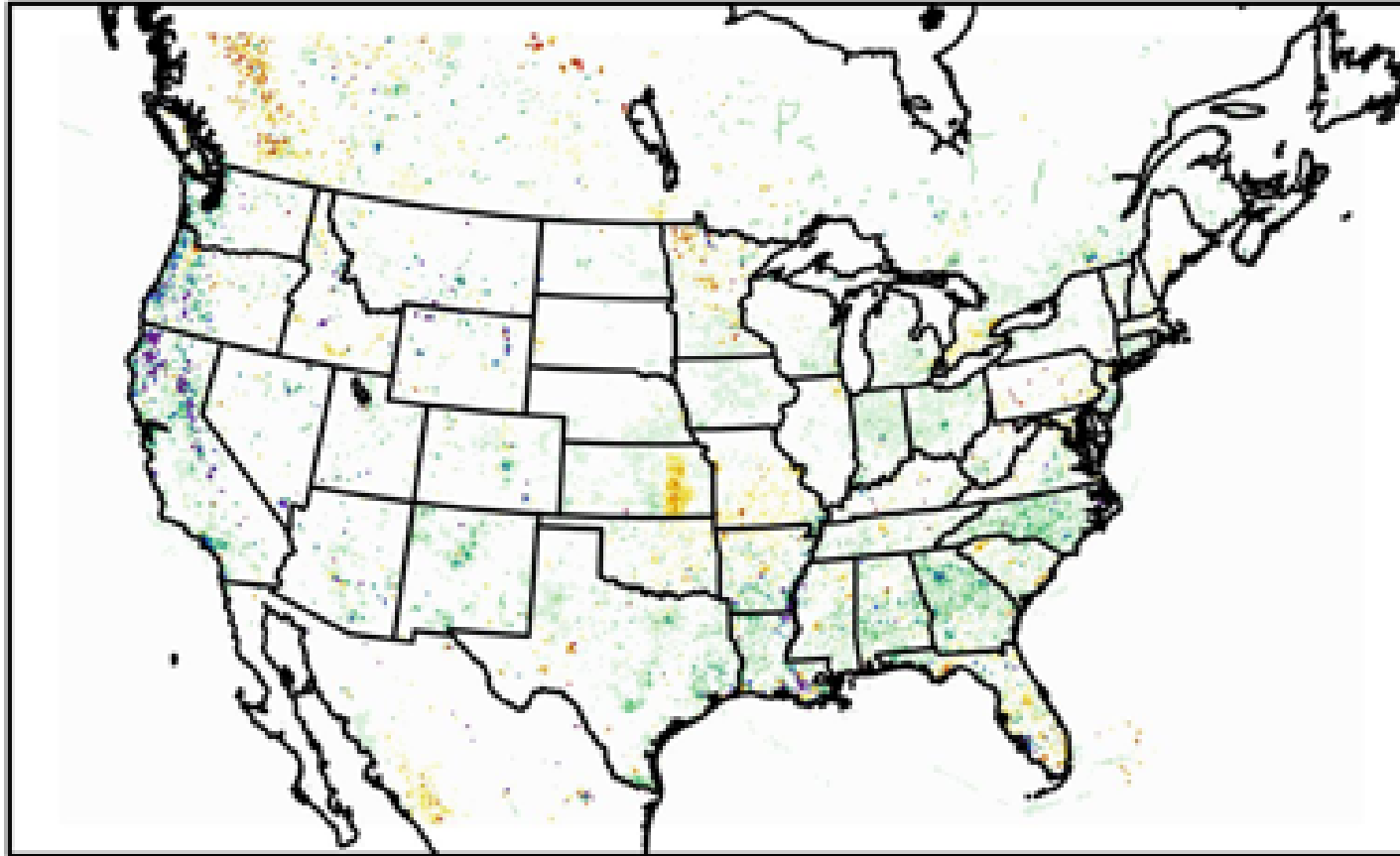
Domain size: 299x459 | Max = 74 at (199, 44)  
Mean: 0.047 | Median: 0.0037

### 2008 EQUATES PM<sub>2.5</sub> Emissions



Domain size: 299x459 | Max = 19 at (174, 38)  
Mean: 0.035 | Median: 0.0016

## EQUATES – ECODEP PM<sub>2.5</sub> 2008 Emissions



Min = -69.4 | Max = 18.4



# Impact of Wildfires on PM<sub>2.5</sub> Seasonal Bias

## December 2017 Southern California wildfires

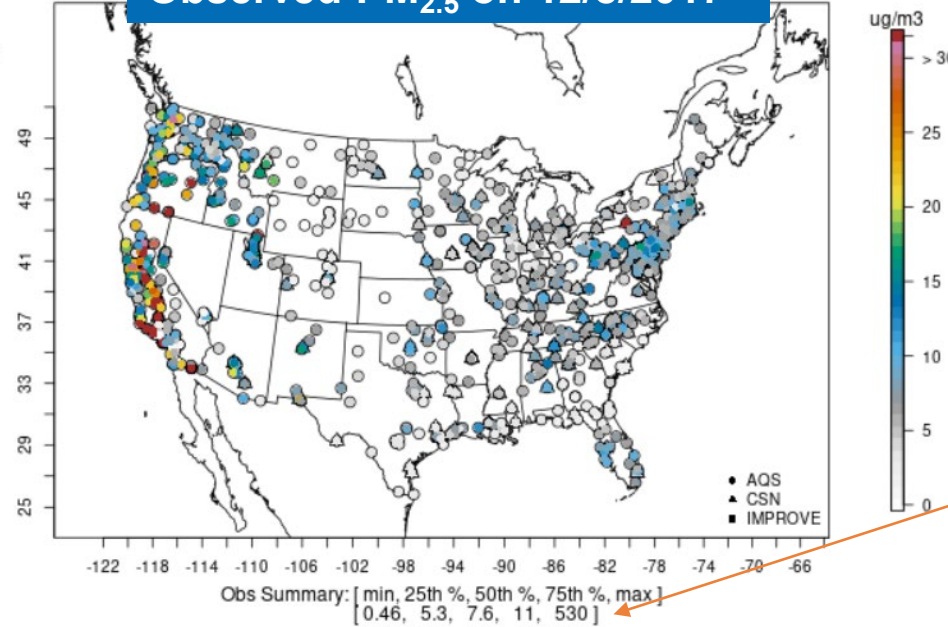


1 Thomas Fire 2 Rye Fire 3 Creek Fire

Satellite image of the smoke from the Thomas Fire and 2 smaller wildfires, on December 5, 2017.

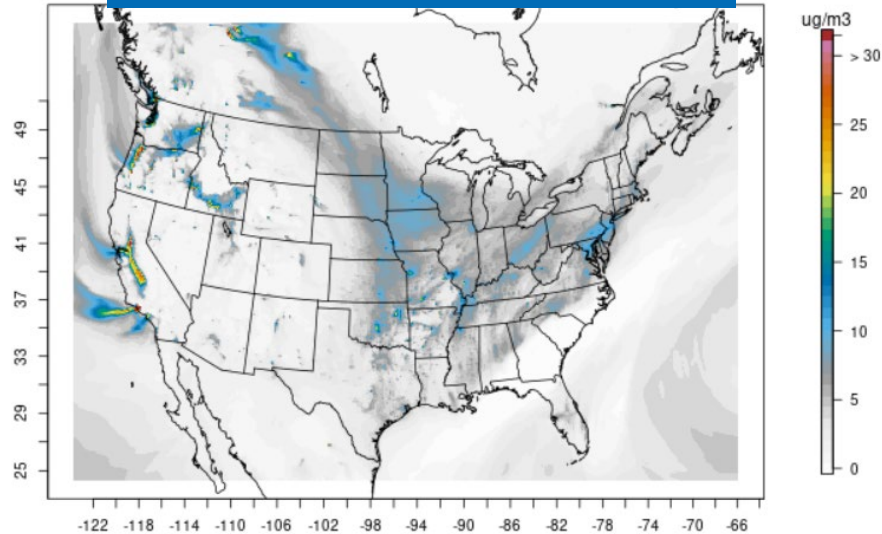
[Source: Wikipedia](#)

## Observed PM<sub>2.5</sub> on 12/8/2017

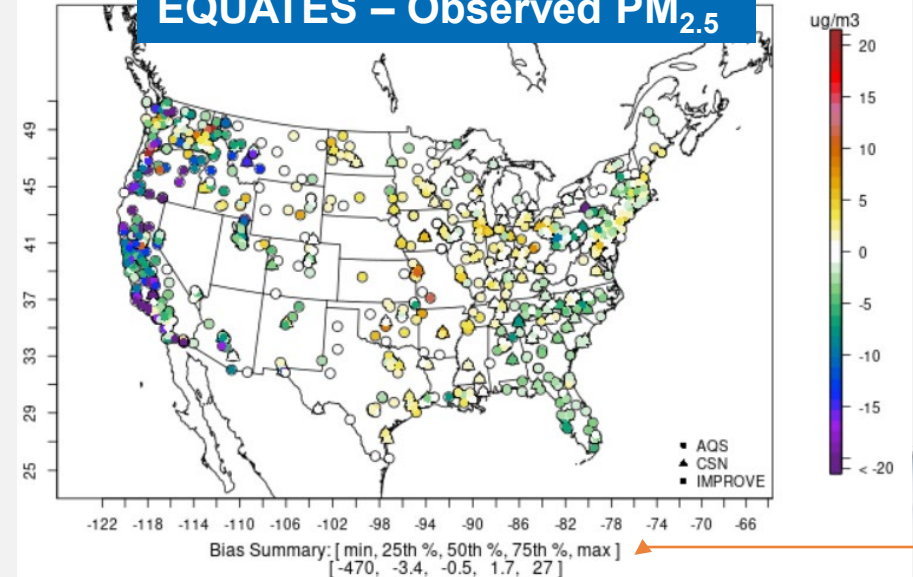


- Largest observed value = 530  $\mu\text{g}/\text{m}^3$
- Largest model bias = -470  $\mu\text{g}/\text{m}^3$

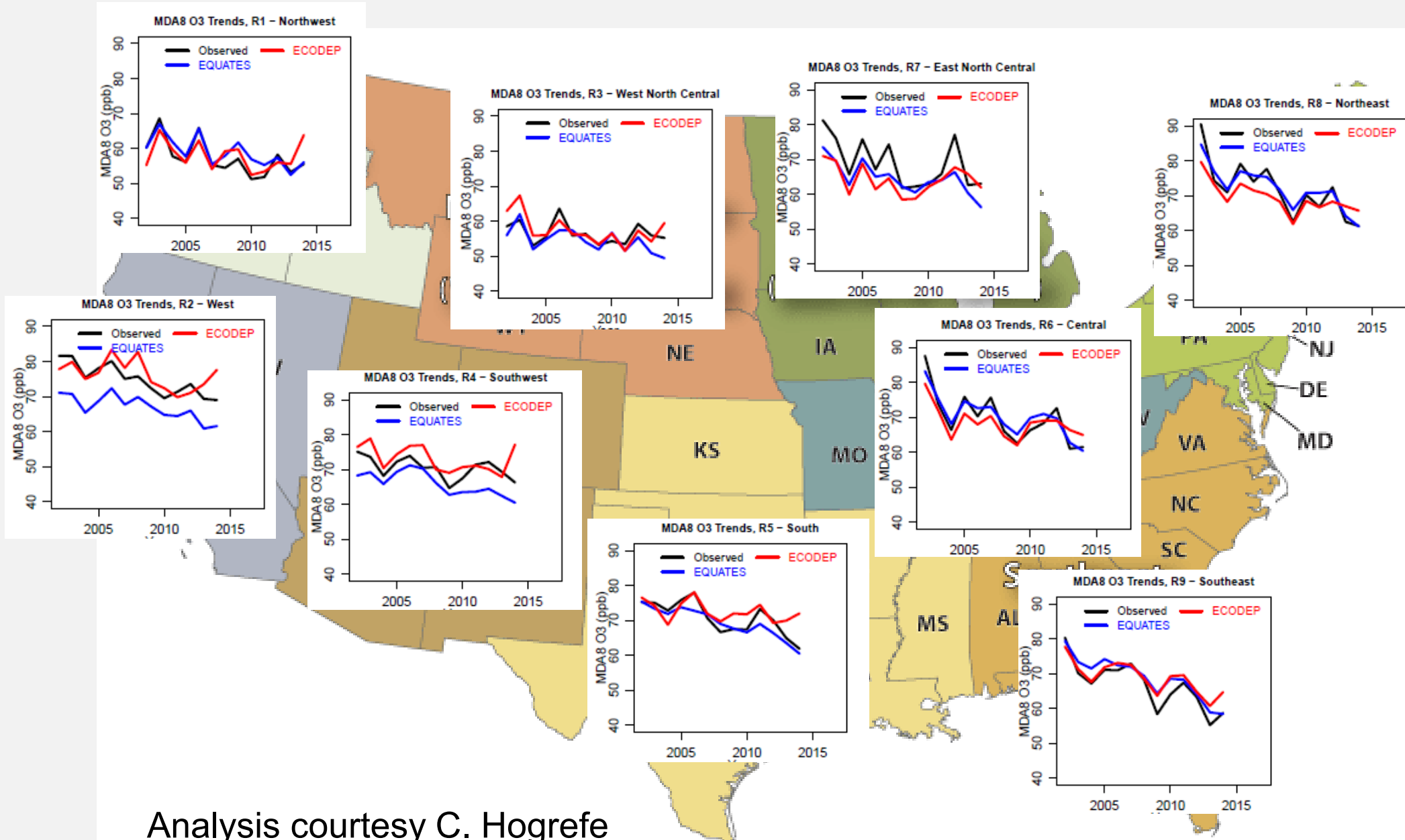
## EQUATES PM<sub>2.5</sub> on 12/8/2017



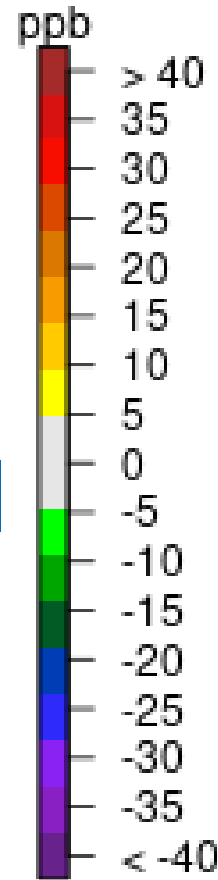
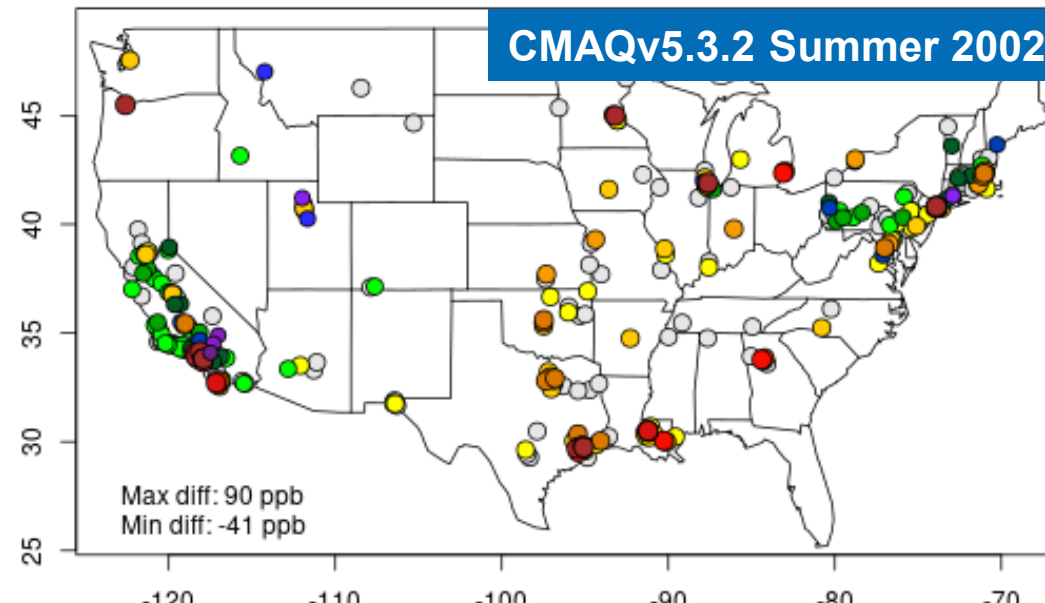
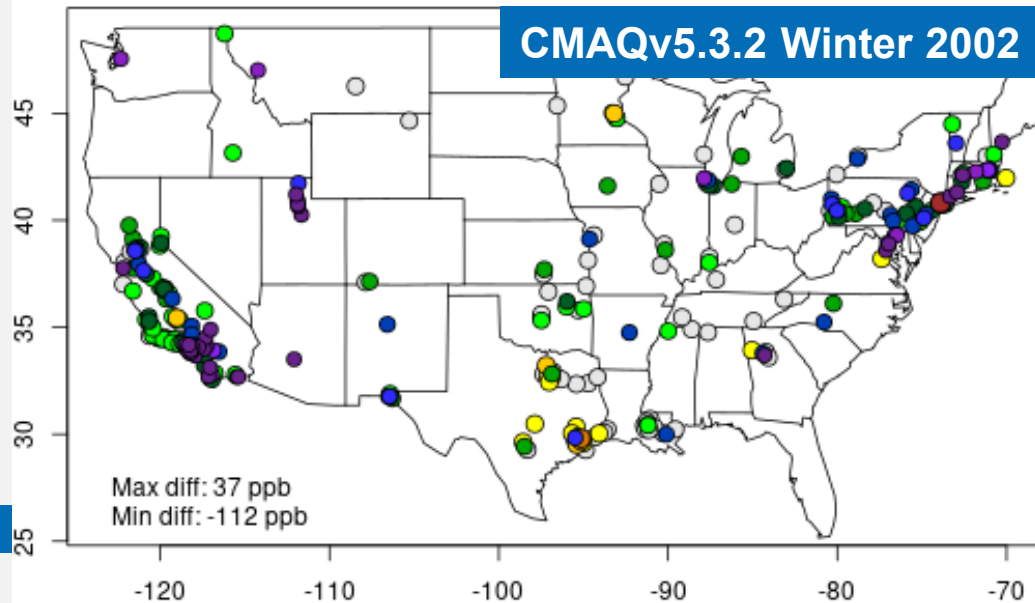
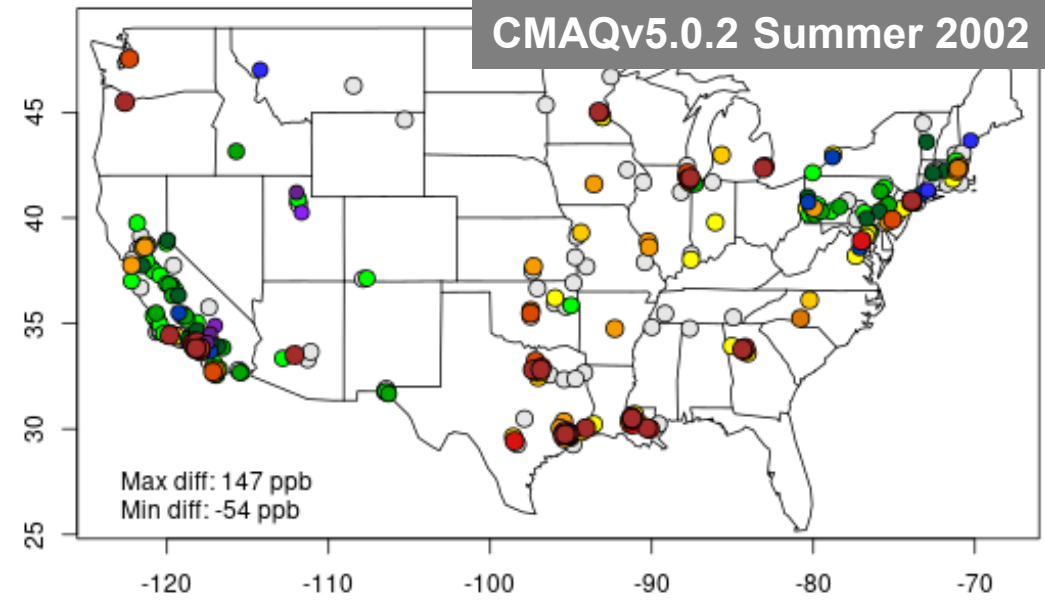
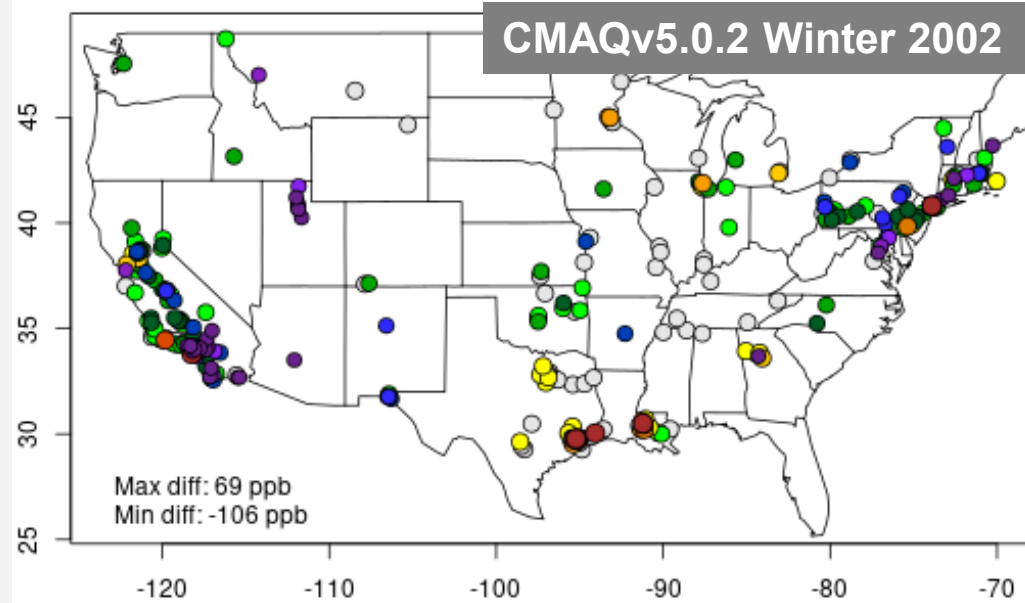
## EQUATES – Observed PM<sub>2.5</sub>



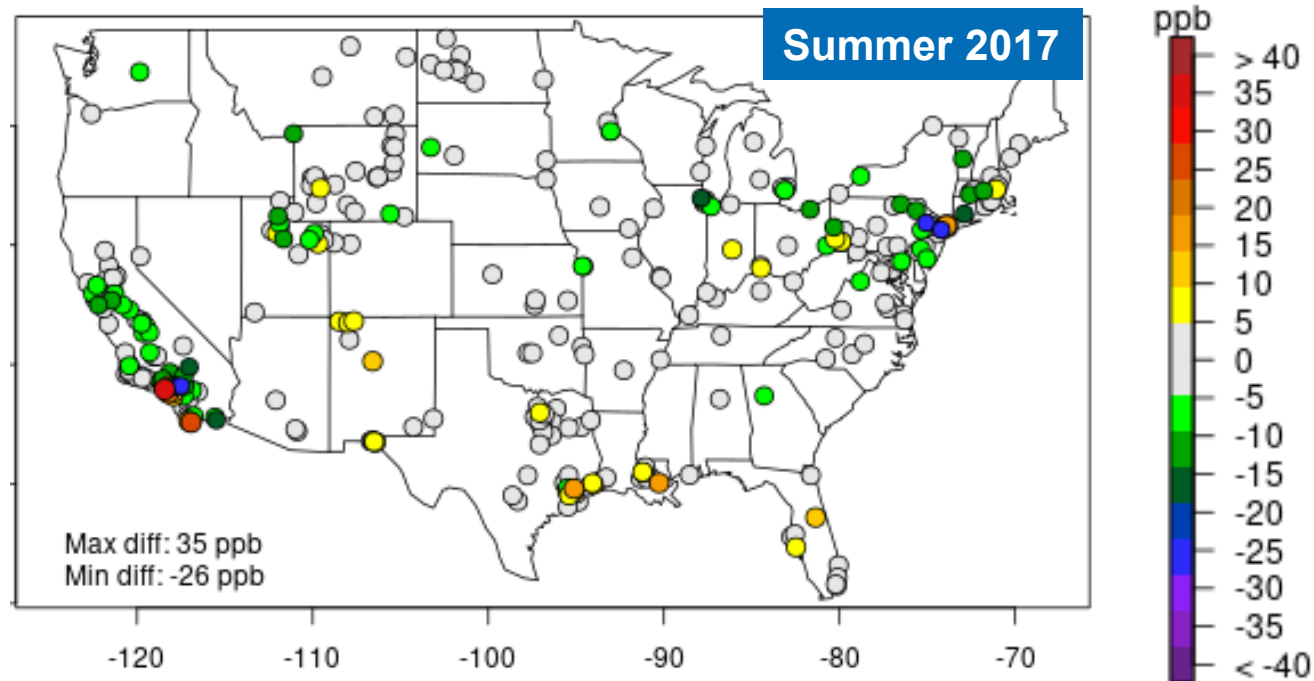
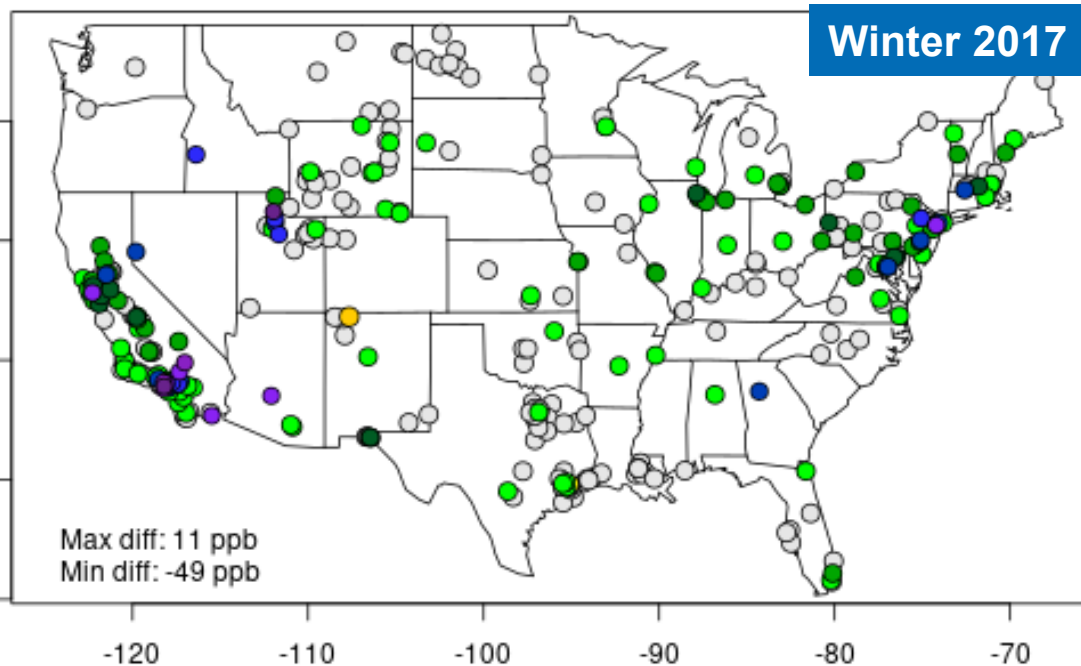
# EQUATES vs ECODEP: Trends in 95<sup>th</sup> Percentile MDA8 O<sub>3</sub> Ozone Season (May –Sept)



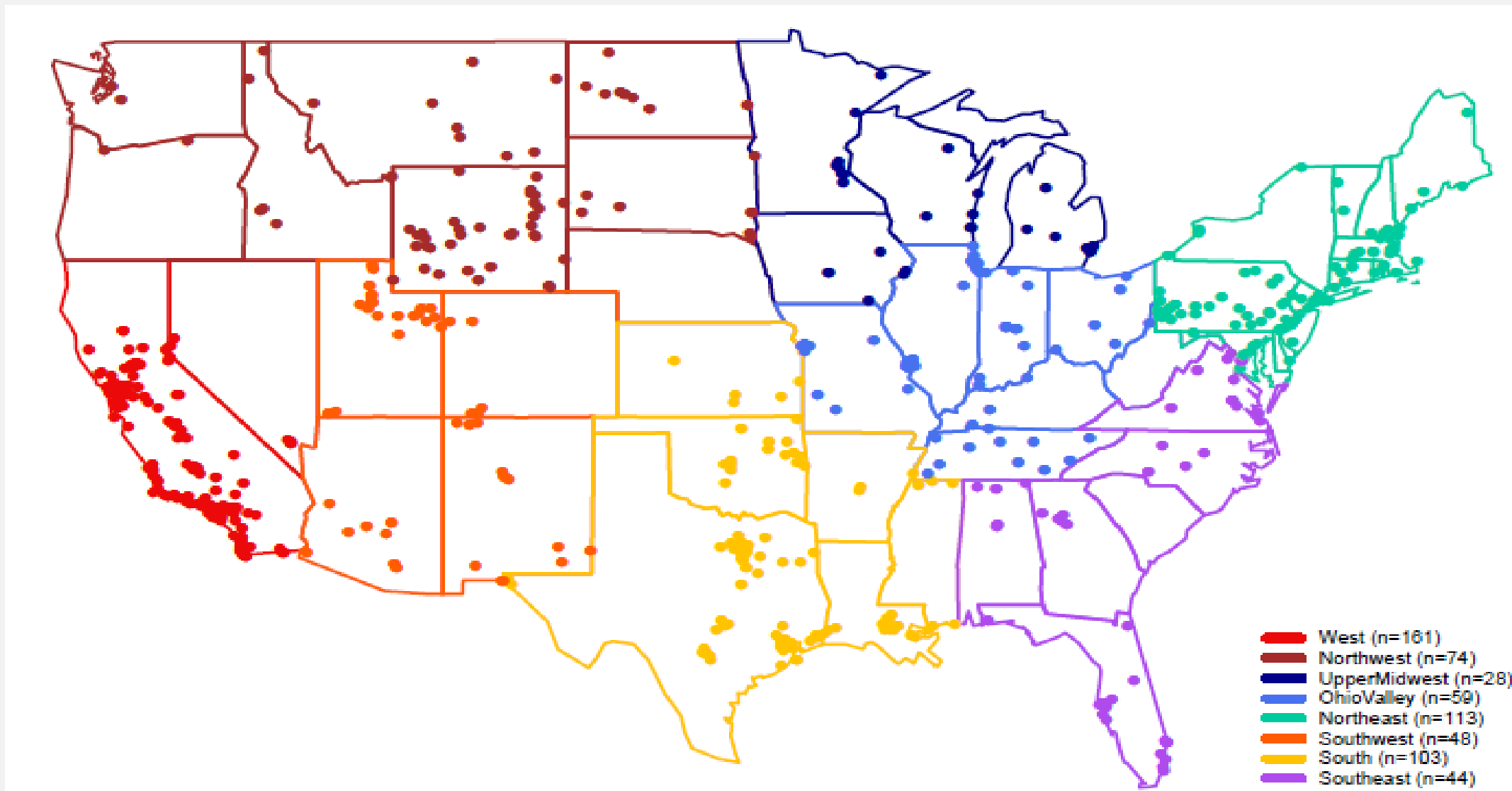
# EQUATES vs ECODEP: 2002 Winter/Summer Bias in 4-9am NO<sub>x</sub>



# EQUATES 2017 Winter/Summer Bias in 4-9am NO<sub>x</sub>



# AQS Sites Grouped by NOAA Climate Regions



# CMAQv5.0.2-CMAQv5.3: 4am-7am NO<sub>x</sub> NMB (%) by Region/Season/Year

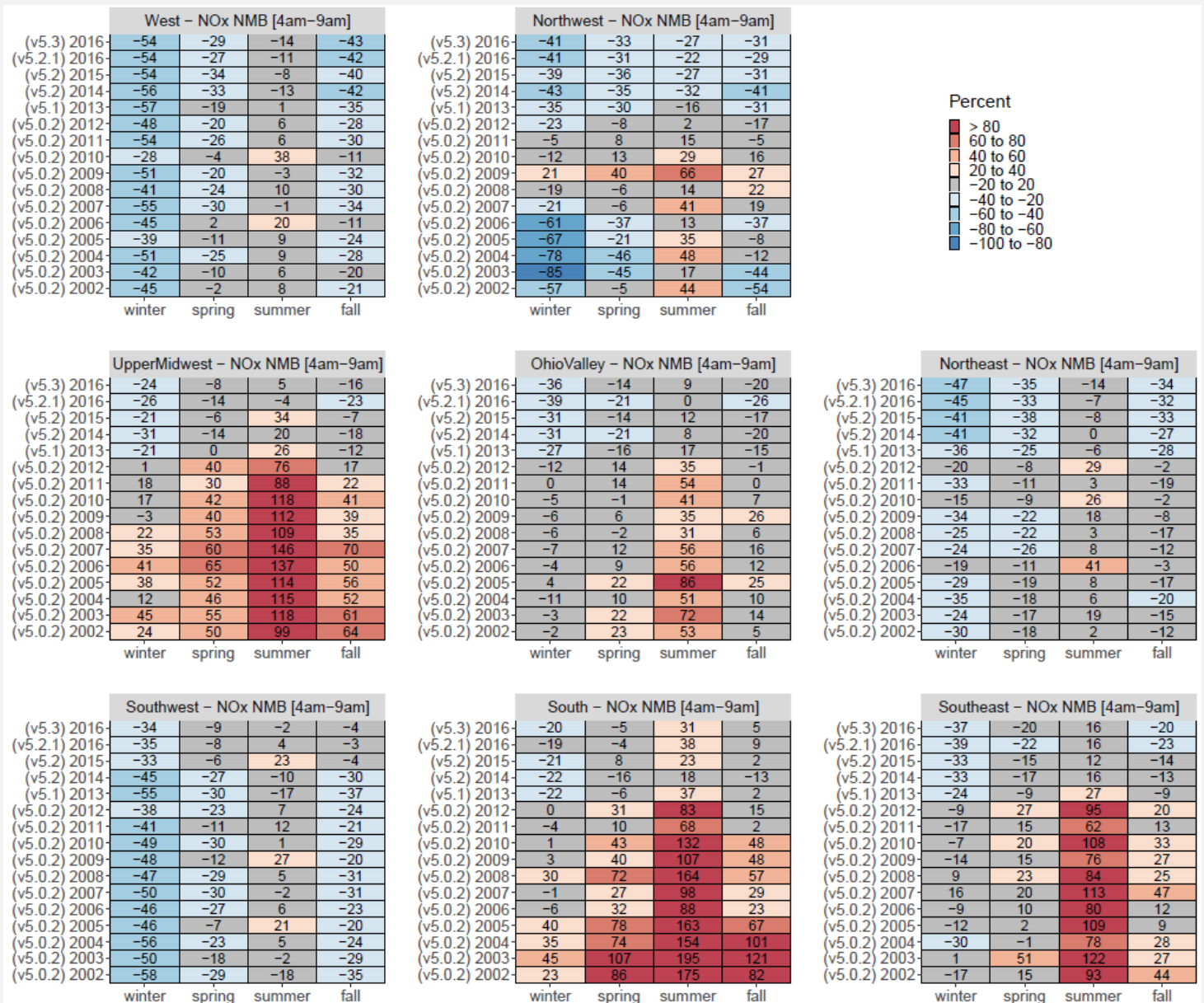


Figure from [Toro et al. \(2021\)](#)  
(Supplemental Figures)

# EQUATES: 4am-7am NO<sub>x</sub> NMB (%) by Region/Season/Year

